Differential Geometry Applied to Crystallography

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Summary

The mathematical facet of modern crystallography is essentially based on analytical geometry, linear algebra as well as group theory. This study endeavours to approach the geometry and symmetry of crystals using the tools furnished by *differential geometry* and the theory of *Lie groups*.

These two branches of mathematics being little known to crystallographers, the pertinent definitions such as *differentiable manifold*, *tangent space* or *metric tensor* or even *isometries on a manifold* together with some important results are given first. The example of euclidean space, taken as riemannian manifold, is treated, in order to show that the affine aspect of this space is not at all an axiom but the consequence of the euclidean nature of the manifold. Attention is then directed to a particular subgroup of the group of euclidean isometries, namely that of translations. This has the property of a Lie group and it turns out that the action of its elements, as well as those of its Lie algebra, plays an important rôle in generating a lattice on a manifold and in its tangent space, too. In particular, it is pointed out that one and only one finite and free module of the Lie algebra of the group of translations can generate both, modulated and non-modulated lattices. This last classification therefore appears continuous rather than black and white and is entirely determined by the parametrisation considered. Since a lattice in a tangent space has the properties of a vector space, it always possesses the structure of a finite, free module, which shows that the assignment of aperiodicity to modulated structures is quite subjective, even unmotivated.

Thanks to the concept of representation of a lattice or a crystal in a tangent space, novel definitions of the notions of *symmetry operation of a space group* and *point symmetry operation*, as well as *symmetry element* and *intrinsic translation* arise; they altogether naturally blend into the framework of differential geometry. In order to conveniently pass from one representation of a crystal in one tangent space to another or to the structure on a manifold, an equivalence relation on the tangent bundle of the manifold is introduced. This relation furthermore allows to extend the concept of symmetry operation to the tangent bundle; this extension furnishes, particularly in the euclidean case, a very practical way of representing symmetry operations of space groups completely devoid of any dependence on an origin, or, in other words, in which each and every point may be considered the origin.

The investigation of the group of translations having being completed, the study of the linear parts of the isometries comes naturally. Based on the fact that the set of linear parts possesses the structure of a Lie group, several results are proven in a rigorous manner, such as the fact that a rotation angle of $\frac{\pi}{3}$ is incompatible with a

three-dimensional cubic lattice. Procedures for determining different crystal systems in function of the type of rotation are laid out by way of the study of orthogonal matrices and their relation to the matrix associated with the type of system.

Finally, the description of a crystal by its diffraction patterns is taken on. It is shown that the general aspect of such a pattern is directly linked to the action of that free and finite module of the Lie algebra of translations which generates a lattice on a manifold. In the case of modulated crystals, it is demonstrated that the appearance of supplementary spots is caused by the geometry, *i.e.* by the parametrisation of the manifold in which the crystal exists and not by the action of the module in the Lie algebra. Thus, there exists a neat separation: the geometrical aspect on the one hand, and the action of the group on the other. As the last topic, other ways of interpreting the diffraction pattern of a modulated structure are laid out in order to argue that mere experimental data do not warrant the uniqueness of a model.

The goal of this study is by no means an attempt at overthrowing existing structural models such as the *superspace*-formalism or at revolutionising the methods for determining structures, but is rather aimed at sustaining that the definition of certain notions becomes thoroughly natural within the appropriate mathematical framework, and, that the term *aperiodicity* assigned to modulated structures no longer has a true meaning.

Résumé

L'aspect mathématique de la cristallographie moderne est principalement basée sur la géométrie analytique, l'algèbre linéaire ainsi que la théorie des groupes. Le présent travail se propose d'aborder la géométrie et la symétrie des cristaux en faisant appel aux outils fournis par la *géométrie différentielle* et la théorie des *groupes de Lie*.

Ces deux domaines mathématiques n'étant que très peu ou pas connu des cristallographes, les notions, telles que *variété différentiable*, *espace tangent* ou *tenseur métrique* ou encore *isométries sur une variété*, sont fournis en premier lieu. L'exemple de l'espace euclidien comme variété riemannienne est traité, afin de montrer que l'aspect affine des isométries de cet espace n'est nullement un axiome mais la conséquence de la nature euclidienne de la variété. L'attention est ensuite focalisée sur un sous-groupe particulier du groupe des isométries euclidiennes, le groupe des translations. Ayant la propriété de groupe de Lie, il s'avère que l'action de ses éléments ainsi que ceux de son algèbre jouent un rôle important dans la génération d'un réseau sur une variété ainsi que dans ses espaces tangents. En particulier, il est mis en évidence qu'un seul et même module libre fini de l'algèbre de Lie du groupe des translations peut générer un réseau non modulé comme modulé, ce dernier aspect dépendant uniquement de la paramétrisation considérée. De par la propriété d'espace vectoriel, un réseau dans un espace tangent a toujours la structure d'un module libre fini, montrant ainsi que l'attribution d'apériodique pour les structures modulées est très subjective, voire non fondée.

Grâce au concept de représentation d'un réseau ou d'un cristal dans un espace tangent, de nouvelles définitions des notions d'*operation de symétrie de groupe d'espace* et *ponctuelle*, ainsi que celles d'*élément de symétrie* et de *translation intrinsèque* peuvent être données et prennent un sens tout à fait naturel dans le cadre de la géométrie différentielle. Afin de pouvoir passer de manière simple de la représentation d'un cristal dans un espace tangent à une autre ou à la structure sur la variété, une relation d'équivalence sur le fibré tangent de la variété est introduite. Cette relation permet en outre d'étendre le concept d'opération de symétrie au fibré tangent, donnant ainsi lieu, dans le cas euclidien en particulier, à une représentation très pratique des opérations de groupes d'espace indépendante de toute origine ou, de manière équivalente, dans laquelle tout point peut être considéré comme point d'origine.

Après l'investigation du groupe des translations vient naturellement l'étude de la partie linéaire des isométries. Exploitant le fait que l'ensemble de ces parties linéaires a une structure de groupe de Lie, plusieurs résultats sont obtenus de manière rigoureuse, comme par exemple le fait que les rotation d'angle $\frac{\pi}{3}$ ne sont pas compatibles avec les réseaux cubiques tridimensionnels. Des marches à suivre pour la détermination des

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différents systèmes cristallins en fonction du type de rotation sont fournies par le biais de l'étude des matrices orthogonales et leur relation avec la matrice associée au type de système.

Finalement, la description d'un cristal au travers de son image de diffraction est abordée. Le fait que l'aspect général d'une telle image, composée de taches dénombrables, soit directement lié à l'action d'un module libre fini de l'algèbre de Lie des translations, celui-là même qui génère un réseau sur un variété, est mis en évidence. Dans le cas des cristaux modulés, il est montré que l'apparition de taches supplémentaires, les *satellites*, est causée par la géométrie, c'est-à-dire la paramétrisation de la variété dans lequel le cristal existe, et non par l'aspect du module dans l'algèbre de Lie; il y a donc bien une séparation nette, l'aspect géométrique d'un côté et l'action d'un groupe de l'autre. En dernier lieu, d'autres pistes quant à l'interprétation d'une image de diffraction d'une structure modulée sont également présentées, afin de montrer que les seules mesures expérimentales ne permettent pas de justifier l'unicité d'un modèle.

Le but de ce travail n'est nullement d'essayer de renverser les modèles existant, comme le formalisme du *superespace*, ainsi que de révolutionner les méthodes de résolution de structures, mais davantage de montrer que la définition de certaines notions devient complètement naturelle lorsqu'un cadre mathématique approprié est utilisé, et ainsi que le terme d'*apériodicité* attribué aux structures modulées n'a plus vraiment de sens.

Mot-clefs : géometrie différentielle, groupes de Lie, symétrie, structures modulées

Contents

Chapter 1

The Concept of Symmetry

Crystallography is originally the mathematically oriented branch of mineralogy, that is the science dedicated to the study of minerals. The term is derived from the greek words κρύσταλλος, which means frozen drop and by extension any solid with some degree of transparency, and γράφο, which means write. A specimen of the mineral quartz is typically a transparent solid which displays shiny smooth plane surfaces intersecting in straight lines and sharp corners. Such characteristics may be used for defining roughly the notion of *crystal*; any solid presenting such features might be called crystal.

1.1   From Kepler to de Wolff

A microscopic definition of crystal calls upon the concept of atomicity and the structure is then considered as a three-dimensional repetition of a pattern composed of atoms. This repetition of a pattern has in fact already been suggested by Johannes Kepler (1571 – 1630) when he was observing the heaven-sent snowflakes; he realised that their hexagonal envelopes also seemed to play a salient role in the densest, planar packing of identical spheres : the concept of a *unit cell* was born. Indeed, the centres of four adjacent spheres form a parallelogram which can be repeated in both dimensions of the considered planar packing. Later, this idea has been adopted and further developed by Jean-Baptiste Louis Romé de L'Isle (1772), René Just Haüy (1784, 1801) and Gabriel Delafosse (1840), who partially foresaw the microscopic definition of a crystal. With the concept of repetition of a pattern, the unit cell, the notion of *three-dimensional periodicity* and *translation symmetry* appeared : the crystal looks the same whether seen from a particular point within one unit cell or another.

Thus, we can think of a crystal as being seamlessly constituted of identical bricks; a direct consequence is that their shape may be left invariant under a rotations only if the angle belongs to $\left\{ \frac{2\pi}{k} \mid k = 1, 2, 3, 4, 6 \right\}$. Rotations of angle $\frac{2\pi}{5}$ and $\frac{2\pi}{k}$, $k \geqslant 7$, are forbidden. All possible bricks, therefore all possible macroscopic crystals, can then be classified in 32 different groups of rotations, known today as crystallographic group of rotations. This result was suggested by Johann Friedrich Christian Hessel in 1830.

If both, Haüy and Delafosse, agreed upon the fact that a crystal is made of a three-dimensional repetition of a block, a unit cell, their viewpoint on its nature was different :

according to the first author, it was a continuum, the second one interpreted it as a discrete set of points, anticipating thus the modern picture of a crystal structure. In the simplest case where a unit cell contains only one point, the whole crystal consists of a set of points called *lattice of translations*. The study of these lattices by Auguste Bravais led him in 1850 to the establishment of the 14 so-called *Bravais lattices*, which classification is compatible with Hessel's.

Thanks to the results of Camille Jordan (1868) on groups of isometries of space, Leonhard Sohncke derived in 1879 all classes of isometries preserving the orientation and leaving a three-dimensional periodic structure invariant; their number was 61. Removing the restriction on orientation-preserving isometries, Evgraf Stepanovitch Fedorov and Artur Schoenflies (1891), as well as William Barlow (1894), independently obtained all classes of isometries leaving a three-dimensional periodic structure invariant up to chirality; the number of these classes, called *space groups*, was 230.

The discovery of X-ray by Wilhelm Konrad Röntgen (1895) and their diffraction by crystals by Walter Friedrich, Paul Knipping and Max von Laue (1912) brought the long sought for confirmation of the atomistic model of matter. Von Laue's conjecture of scattering of X rays by crystals extended Thomson's work on the elastic scattering of electromagnetic radiation by the electron (1898). The shape of the diffraction pattern of a crystal, characterised by sharp spots lying on the nodes of a three-dimensional lattice of translation (in the same meaning as those considered by Bravais), the so-called *reciprocal lattice* (see chapter 5), was an evidence in favour of the three-dimensional periodicity, that is the repetition on three dimensions of a brick.

Diffraction by X-rays, as well as by neutrons or electrons, is a powerful tool for extracting information about the structure of a crystal. On one hand, the shape of the reciprocal lattice provides characteristics of the unit cell; on the other hand, the decoration of the unit cell, that is the position of the atoms in the cell, can be deduced from the distribution of the intensities of the spots; moreover, some information about the symmetry of the cell is obtained, as the rotations leaving a unit cell invariant also figure in the diffraction pattern.

Saying that the spots in the diffraction pattern lie all on a three-dimensional lattice of translation amounts to saying that their position can be located or indexed with three integer coordinates. However, in the course of the twentieth century, several major discoveries overthrew the concepts and definitions established in the previous hundred years. Among all investigations done, three of them merit to be placed in exergue. First, the investigation of sodium carbonate γ-Na_2CO_3 by Pieter Maarten de Wolff and coworkers showed extra spots in its diffraction pattern, which could not be indexed by only three integer coordinates as it was usually done [BVdW64]. Second, the discovery of the compounds $Cr_{11}Ge_{19}$, $Mo_{13}Ge_{23}$ and $V_{17}Ge_{31}$ by Hans Nowotny and coworkers in 1967 put forward the existence of the so-called intergrowth crystals, consisting in the interpenetration of two independent lattices of translation composed of different atoms and the dimensions of which are incommensurate [VPNW67]. Finally, the study of an aluminium-manganese alloy by D. Shechtman, J. W. Cahn and coworkers showed sharp spots in a diffraction pattern presenting an invariance under a rotation of angle $\frac{2\pi}{5}$, what was not consistent with one aspect in the definition of a crystal : the three-dimensional

repetition of a unit cell [SBGC84].

The consequence of these discoveries was to reconsider the definition of a crystal and propose a new one including these compounds with special properties. The question was, and still is, how to proceed...

1.2 Current Models

In crystallography, the space in which a crystal exists is called *direct space* and the space of its diffraction pattern *reciprocal space*. The direct space has the structure of a so-called *point space* $\mathcal{E}$, the properties of which are mainly dictated by an *associated vector space* V. This space is endowed with a scalar product, it is a pre-Hilbert space, and is connected to the point space in the following way : to any two points p and q of $\mathcal{E}$ corresponds a vector $pq \doteq r$ of V. Lengths between points and angles between lines are calculated *via* the scalar product in V [Won02]. Isometries in $\mathcal{E}$ are assumed to be affine maps, consisting of a *linear* or *matrix part* and a *translation part*; a *symmetry operation* of a geometrical object is a particular isometry which leaves the object invariant. In this frame, a lattice of translation, that is a repetition in three dimensions of a brick, the unit cell, is nothing else than a finite free $\mathbb{Z}$-module, which can be noted

$$\left\{ \sum_{j=1}^{3} \lambda^j \, a_j \;\middle|\; \lambda^j \in \mathbb{Z},\, 1 \leqslant j \leqslant 3 \right\} \,,$$

where the vectors a_1, a_2 and a_3 form a basis of V, or, equivalently, in matrix notation :

$$\left\{ B\,\lambda = \left((B\,\lambda)^1;\, (B\,\lambda)^2;\, (B\,\lambda)^3 \right) \;\middle|\; \lambda = (\lambda^1;\, \lambda^2;\, \lambda^3) \in \mathbb{Z}^3 \right\} \,.$$

where $B \in \mathrm{GL}_3(\mathbb{R})$ is a matrix describing the shape of the module. The concept of three-dimensional repetition is expressed by the property that the sum of any two elements of such a module is also an element of this module; this fact constitutes a way of characterising the periodicity of a crystal; a way commonly adopted in crystallography.

About ten years after the investigation of sodium carbonate by Pieter de Wolff and coworkers, the structure of this compound was successfully refined on the assumption that it is a usual three-dimensional periodic structure, which is distorted by a periodic wave function of the position with a sinusoidal shape [dW74]. This idea was assuredly inspired by the work of V. Daniel and H. Lipson [DL43], who observed that a regular deformation of the original cubic lattice in the alloy $\mathrm{Cu_4FeNi_3}$ caused additional spots in its diffraction pattern.

The main consequence of this periodic deformation is that the structure cannot *a priori* be considered as a three-dimensional repetition of a brick, there does not exist an associated lattice with a finite free $\mathbb{Z}$-module structure, the crystal cannot be considered periodic, in the crystallographic sense. Nevertheless, periodicity is a concept cherished by crystallographers, in particular by Pieter de Wolff. In order to recover it, he had the idea to consider a point space of dimension higher than three, in which the crystal exists; in other words, he gave birth to the *superspace* formalism. An overview of this model, which was further developed by A. Janner, T. W. J. Janssen and others, is

presented here in order to understand its essential features (for more information, see the references [JJLVdW02, JCdB07, vS95, vS07]).

The reciprocal space, in which the diffraction pattern of a structure exists, can be seen as the space $\mathbb{R}^3$ consisting in the cartesian product of three copies of the real field $\mathbb{R}$. Moreover, these three copies are supposed to be orthogonal between themselves, with respect to the usual Euclidean scalar product. The canonical basis $\{e^1; e^2; e^3\}$ of $\mathbb{R}^3$, where $e^1 = (1; 0; 0)$, $e^2 = (0; 1; 0)$ and $e^3 = (0; 0; 1)$ is then an orthonormal basis. The diffraction pattern of sodium carbonate presents main spots lying on the nodes of a lattice of translation, that is on points of a finite free $\mathbb{Z}$-module generated by three independent vectors a^{*1}, a^{*2} and a^{*3} of which the coordinates with respect to the canonical basis are :

$$a^{*1} = \sum_{j=1}^{3} \bar{b}^1_j \, e^j \; , \qquad a^{*2} = \sum_{j=1}^{3} \bar{b}^2_j \, e^j \; , \qquad a^{*3} = \sum_{j=1}^{3} \bar{b}^3_j \, e^j \; , \qquad (1.2.1)$$

where $B^{-1} \doteq (\bar{b}^i_j)^3_{i,j=1}$ is an invertible 3×3 matrix. Concerning the additional spots, their coordinates can be obtained by adding to the coordinates of main spots an integer multiple of a vector ξ, given with respect to the canonical basis by :

$$\xi = \sum_{j=1}^{3} \xi_j \, e^j \; . \qquad (1.2.2)$$

Pieter de Wolff's fundamental idea was to consider this vector ξ as the result of a projection of a vector X living in a four dimensional vector space. $\mathbb{R}^3$ is extended to $\mathbb{R}^4 = \mathbb{R}^3 \times \mathbb{R}$, with $\mathbb{R}$ considered to be orthogonal to $\mathbb{R}^3$. The canonical vectors e^1, e^2, e^3 and e^4 of $\mathbb{R}^4$, composed of the three vectors of the canonical basis of $\mathbb{R}^3$, with a 0 as the fourth component, $e^1 = (1; 0; 0; 0)$, $e^2 = (0; 1; 0; 0)$, $e^3 = (0; 0; 1; 0)$, and the fourth vector $e^4 = (0; 0; 0; 1)$. X can be written as :

$$X = \sum_{j=1}^{3} \xi_j \, e^j + \xi_\perp \, e^4 \; , \qquad (1.2.3)$$

where $\xi_\perp$ is an arbitrary non-zero real number. Then, a^{*1}, a^{*2}, a^{*3}, and X form a basis which can be expressed from the canonical basis of $\mathbb{R}^4$ by the relation :

$$\begin{pmatrix} a^{*1} \\ a^{*2} \\ a^{*3} \\ X \end{pmatrix} = \begin{pmatrix} \bar{b}^1_1 & \bar{b}^1_2 & \bar{b}^1_3 & 0 \\ \bar{b}^2_1 & \bar{b}^2_2 & \bar{b}^2_3 & 0 \\ \bar{b}^3_1 & \bar{b}^3_2 & \bar{b}^3_3 & 0 \\ \xi_1 & \xi_2 & \xi_3 & \xi_\perp \end{pmatrix} \begin{pmatrix} e^1 \\ e^2 \\ e^3 \\ e^4 \end{pmatrix} \; . \qquad (1.2.4)$$

where the 4×4 matrix, noted $\underline{B}^{-1}$ may be written in a compact way as :

$$\underline{B}^{-1} = \left(\begin{array}{c|c} B^{-1} & 0 \\ \hline {}^t\xi & \xi_\perp \end{array} \right) \; , \qquad (1.2.5)$$
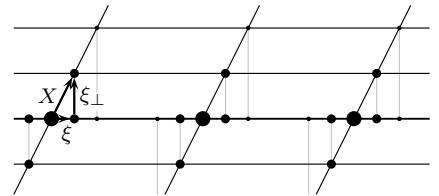
where 0 is a 3×1 block containing only 0. As $\underline{B}^{-1}$ is not orthogonal, $\{a^{*1}; a^{*2}; a^{*3}; X\}$ is not orthonormal. However, the parallelepiped generated by these four vectors does not have an arbitrary shape, as it must satisfy certain symmetry rules which will be explained further.

The diffraction pattern of a crystal structure is mathematically described by the Fourier transform (see chapter 5 and appendix C); the intensities of the spots correspond to the square modulus of the Fourier transform of the electron density. In a modulated structure, this density can be written as (see equation 5.1.7 in chapter 5 and article [JJ87]) :

$$\rho(r) \;=\; \frac{1}{(2\,\pi)^3} \int_{\mathbb{R}^n} \sum_{\ell \in \mathbb{Z}^3} \sum_{m \in \mathbb{Z}} \varrho(k;\, m)\, \delta\Big(k - 2\,\pi\,\big({}^{\mathrm{t}}(B^{-1})\,\ell - m\,\xi\big)\Big) \exp(-\mathrm{i}\,k \cdot r)\, \mathrm{d}^n k \;=\;$$

$$=\; \frac{1}{(2\,\pi)^3} \sum_{\ell \in \mathbb{Z}^3} \sum_{m \in \mathbb{Z}} \varrho(\ell;\, m)\, \exp\Big(-2\,\pi\,\mathrm{i}\,\big({}^{\mathrm{t}}(B^{-1})\,\ell - m\,\xi\big) \cdot r\Big)\;, \tag{1.2.6}$$

where ϱ corresponds mostly to the Fourier transform of ρ over a unit cell, r is a three-dimensional variable, corresponding to the position-vector in $\mathbb{R}^3$, and $\cdot$ is the Euclidean scalar product. The generalised Dirac function δ present in the first line of this expression illustrates the fact that the diffraction pattern is composed of sharp spots on the nodes of the lattice $2\,\pi\,\Lambda^*$, where Λ^* is the finite free $\mathbb{Z}$-module generated by a^{*1}, a^{*2} and a^{*3}, and additional (satellite) spots about each main spot, according to the direction given by the wave vector ξ; note that the factor $2\,\pi$ can be removed when introducing the variable $\bar{k} = \frac{k}{2\,\pi}$. Introducing the fourth parameter $\xi_\perp$ and then also an additional variable r^4, we obtain an augmented electron density on $\mathbb{R}^4$:

$$\rho^{(4)}(r;\, r^4) = \frac{1}{(2\,\pi)^3} \sum_{\ell \in \mathbb{Z}^3} \sum_{m \in \mathbb{Z}} \varrho(\ell;\, m)\, \exp\Big(-2\,\pi\,\mathrm{i}\,\big({}^{\mathrm{t}}(B^{-1})\,\ell - m\,\xi\big) \cdot r + 2\,\pi\,\mathrm{i}\,m\,\xi_\perp\,r^4\Big)\;, \tag{1.2.7}$$

which is equal to $\rho(r)$ in the case $r^4 = 0$. $\rho^{(4)}$ corresponds to the electron density of a structure in four dimensions, where the atoms are lines, that is smooth or piecewise smooth curves, and no more points (a one-dimensional example is shown in figure 2.6); it has a four-dimensional periodicity, in the sense that it corresponds to a four-dimensional repetition of a four-dimensional decorated brick. Indeed, let

$$\Lambda^{(4)} = \{\underline{B}\,\lambda^{(4)} \mid \lambda^{(4)} = (\lambda^1;\, \lambda^2;\, \lambda^3;\, \lambda^4),\, \lambda^j \in \mathbb{Z},\, 1 \leqslant j \leqslant 4\}\;,$$

where :

$$\underline{B} = \begin{pmatrix} b^1{}_1 & b^1{}_2 & b^1{}_3 & 0 \\ b^2{}_1 & b^2{}_2 & b^2{}_3 & 0 \\ b^3{}_1 & b^3{}_2 & b^3{}_3 & 0 \\ -\frac{({}^{\mathrm{t}}\xi\,B)_1}{\xi_\perp} & -\frac{({}^{\mathrm{t}}\xi\,B)_1}{\xi_\perp} & -\frac{({}^{\mathrm{t}}\xi\,B)_1}{\xi_\perp} & \frac{1}{\xi_\perp} \end{pmatrix} = \left(\begin{array}{c|c} B & 0 \\ \hline -\frac{{}^{\mathrm{t}}\xi\,B}{\xi_\perp} & \frac{1}{\xi_\perp} \end{array} \right) \quad, \tag{1.2.8}$$

with $B = (b^i{}_j)^3_{i,j=1}$ the inverse matrix of B^{-1}. Then, for any

$$r'^{(4)} = r^{(4)} + \underline{B}\,\lambda\;,$$

where :

$$r^{(4)} = (r^1;\, r^2;\, r^3;\, r^4) \doteq (r;\, r^4) \ ,$$

$$r'^{(4)} = (r'^1;\, r'^2\,;\, r'^3;\, r'^4) \doteq (r'\,;\, r'^4) \ ,$$

$$\lambda^{(4)} \doteq (\lambda^1;\, \lambda^2;\, \lambda^3;\, \lambda^4) \doteq (\lambda\,;\, \lambda^4) \ ,$$

we have :

$$
\rho^{(4)}(r';\, r'^4) \;=\; \frac{1}{(2\,\pi)^3} \sum_{\ell \in \mathbb{Z}^3} \sum_{m \in \mathbb{Z}} \varrho(\ell;\, m) \exp\!\Big(-2\,\pi\,\mathrm{i}\,\big(\,^{\mathrm{t}}(B^{-1})\,\ell - m\,\xi\big)\cdot r + 2\,\pi\,\mathrm{i}\,m\,\xi_\perp\, r^4 \Big) \cdot
$$

$$
\cdot \exp\big(2\,\pi\,\mathrm{i}\,(\ell \cdot \lambda - m\,\lambda^4)\big) \;=\;
$$

$$
=\; \frac{1}{(2\,\pi)^3} \sum_{\ell \in \mathbb{Z}^3} \sum_{m \in \mathbb{Z}} \varrho(\ell;\, m) \exp\!\Big(-2\,\pi\,\mathrm{i}\,\big(\,^{\mathrm{t}}(B^{-1})\,\ell - m\,\xi\big)\cdot r + 2\,\pi\,\mathrm{i}\,m\,\xi_\perp\, r^4 \Big) \ ,
$$

as $\ell \cdot \lambda - m\,\lambda^4$ is an integer number. The invariance of $\rho^{(4)}$ under the addition of an element of $\Lambda^{(4)}$ to $r^{(4)}$ shows the four-dimensional periodicity of the extended structure. To this structure is then associated a lattice generated by the four vectors :

$$
{}_4a_1 = \sum_{j=1}^{3} \left(e_j - e_4\, \frac{\xi_j}{\xi_\perp} \right) b^j_{\ 1} \ , \tag{1.2.10a}
$$

$$
{}_4a_2 = \sum_{j=1}^{3} \left(e_j - e_4\, \frac{\xi_j}{\xi_\perp} \right) b^j_{\ 2} \ , \tag{1.2.10b}
$$

$$
{}_4a_3 = \sum_{j=1}^{3} \left(e_j - e_4\, \frac{\xi_j}{\xi_\perp} \right) b^j_{\ 3} \ , \tag{1.2.10c}
$$

$$
{}_4a_4 = \frac{e_4}{\xi_\perp} \quad , \tag{1.2.10d}
$$

where $\{e_1;\, e_2;\, e_3;\, e_4\}$ is the canonical orthonormal basis of the vector space $\mathbb{R}^4$. The expression of ${}_4a_1,\ {}_4a_2,\ {}_4a_3$ and ${}_4a_4$ can be obtained from a matrix multiplication :

$$
\big(\begin{array}{cccc} {}_4a_1 & {}_4a_2 & {}_4a_3 & {}_4a_4 \end{array} \big) = \big(\begin{array}{cccc} e_1 & e_2 & e_3 & e_4 \end{array} \big)
\begin{pmatrix}
b^1_{\ 1} & b^1_{\ 2} & b^1_{\ 3} & 0 \\
b^2_{\ 1} & b^2_{\ 2} & b^2_{\ 3} & 0 \\
b^3_{\ 1} & b^3_{\ 2} & b^3_{\ 3} & 0 \\
-\frac{(\,^{\mathrm{t}}\xi\, B)_1}{\xi_\perp} & -\frac{(\,^{\mathrm{t}}\xi\, B)_1}{\xi_\perp} & -\frac{(\,^{\mathrm{t}}\xi\, B)_1}{\xi_\perp} & \frac{1}{\xi_\perp}
\end{pmatrix} \ .
\tag{1.2.11}
$$

Writing ${}_4a^{*1} \doteq a^{*1}$, ${}_4a^{*2} \doteq a^{*2}$, ${}_4a^{*3} \doteq a^{*3}$ and ${}_4a^{*4} \doteq X$, we derive the property :

$$
{}_4a^{*i} \cdot {}_4a_j = \delta^i_{\ j} \ , \qquad 1 \leqslant i,j \leqslant 4 \ . \tag{1.2.12}
$$

A three-dimensional crystal distorted by one periodic wave function of the position can thus be seen as a four-dimensional structure which has four-dimensional periodicity

in the sense that it corresponds to a repetition in four dimensions of a decorated brick, the unit cell. Thus, as in the three-dimensional case, symmetry operations of four-dimensional crystals, that is isometries leaving the crystal invariant, consist in a matrix part $\underline{F}$ and a translation part $s^{(4)}$; a position-vector $r^{(4)}$ in four dimensions, written in components as a column-matrix, is transformed into :

$$r'^{(4)} = \underline{F}\, r^{(4)} + s^{(4)} \; ; \tag{1.2.13}$$

when referred to an orthonormal basis, $\underline{F}$ is orthogonal. It must be borne in mind, however, that a three-dimensional modulated crystal still lives in three dimensions and corresponds to a section of the extended four-dimensional structure. In other words, the real crystal exists in $\mathbb{R}^3$ which is a part of $\mathbb{R}^4 = \mathbb{R}^3 \times \mathbb{R}$; in the language of vector spaces, $\mathbb{R}^4$, noted V_{ss} and called four-dimensional *superspace*, can be seen as a direct sum :

$$V_{\mathrm{ss}} = V_{\mathrm{ext}} \oplus V_{\mathrm{int}} \; , \tag{1.2.14}$$

where

$$V_{\mathrm{ext}} = \{v^{(4)} = (v^1;\, v^2;\, v^3;\, v^4) \in \mathbb{R}^4 \mid v^4 = 0\}$$

is called *external space* and

$$V_{\mathrm{int}} = \{v^{(4)} = (v^1;\, v^2;\, v^3;\, v^4) \in \mathbb{R}^4 \mid v^1 = v^2 = v^3 = 0\}$$

is called *internal space*. As $\mathbb{R}^4$ is considered as four orthogonal copies of $\mathbb{R}$, then in particular $\mathbb{R}$ is orthogonal to $\mathbb{R}^3$ and the direct sum is orthogonal. In order that the three-dimensional modulated structure be left invariant under a symmetry operation of the extended four-dimensional structure, the matrix part $\underline{F}$ of the operation must leave V_{ext} and V_{int} invariant. With respect to the canonical orthonormal basis $\{e_1;\, e_2;\, e_3;\, e_4\}$ of $\mathbb{R}^4$, $\underline{F}$ is orthogonal and composed of a 3×3 block F_{ext} and a 1×1 block F_{int} which are both orthogonal as well :

$$\underline{F} = \left(\begin{array}{c|c} F_{\mathrm{ext}} & 0 \\ \hline 0 & F_{\mathrm{int}} \end{array} \right) \tag{1.2.16}$$

As $F_{\mathrm{int}} \in \mathrm{O}_1(\mathbb{R})$, it can be only equal to ± 1. As it will be shown in chapter 5, the diffraction pattern of a modulated structure is left invariant under any linear map corresponding to the matrix part F of a symmetry operation of the three-dimensional average structure, that is the structure non-distorted by the modulation. In the expression above, the matrix F_{ext} then corresponds to a certain matrix part F of a symmetry operation of the average structure.

A consequence of this invariance of the diffraction pattern under the matrix part F is that main spots are transformed into main spots and additional (satellite) spots into additional ones. The translation of this condition to the diffraction pattern extended to four dimensions is that the matrix operations leaving this latter invariant can be only of the form 1.2.16 with respect to the canonical orthonormal basis of $\mathbb{R}^4$; immiscibility of main and satellite spots goes in pair with the invariance of the three-dimensional

reciprocal space $\mathbb{R}^3$ and the orthogonal additional one $\mathbb{R}$. Under the action of $\underline{F}$, the position-vector $v^{(4)}$ of any spot, which can be written as

$$v^{(4)} = {}^{\mathrm{t}}\ell^{(4)} \,{}_4a^* \,, \qquad (1.2.17)$$

where ${}_4a^* = (a^*; X) = (a^{*1}; a^{*2}; a^{*3}; X)$, $\ell^{(4)} = (\ell; m) = (\ell_1; \ell_2; \ell_3; m)$, $m \in \mathbb{Z}$, $\ell = (\ell_1; \ell_2; \ell_3) \in \mathbb{Z}^3$, is transformed into the position-vector :

$$v'^{(4)} = {}^{\mathrm{t}}\ell^{(4)} \underline{B}^{-1} \underline{F}^{-1} \underline{B} \,{}_4a^* \,. \qquad (1.2.18)$$

The matrix $\underline{B}\,\underline{F}^{-1}\underline{B}^{-1}$ is the representation of the orthogonal matrix $\underline{F}^{-1}$ in the basis $\{a^{*1}; a^{*2}; a^{*3}; X\}$; it is justified by the fact that $v^{(4)}$ expressed with respect to the canonical orthonormal basis vectors ${}_4e = (e^1; e^2; e^3; e^4)$ is :

$$v^{(4)} = {}^{\mathrm{t}}\ell^{(4)} \,{}_4a^* = {}^{\mathrm{t}}\ell^{(4)} \underline{B}^{-1} \underline{B} \,{}_4a^* = {}^{\mathrm{t}}\ell^{(4)} \underline{B}^{-1} \,{}_4e^* \,,$$

where ${}^{\mathrm{t}}(\underline{B}^{-1})\,\ell^{(4)}$ is the column-vector containing the components of $v^{(4)}$ with respect to the orthonormal basis $\{e^1; e^2; e^3; e^4\}$. It is transformed into $\underline{F}\,{}^{\mathrm{t}}(\underline{B}^{-1})\,\ell^{(4)}$, so that :

$$v'^{(4)} = {}^{\mathrm{t}}(F\,{}^{\mathrm{t}}(\underline{B}^{-1})\,\ell^{(4)})\,{}_4e^* = {}^{\mathrm{t}}\ell^{(4)} \underline{B}^{-1}\,{}^{\mathrm{t}}\underline{F}\,{}_4e^* = {}^{\mathrm{t}}\ell^{(4)} \underline{B}^{-1}\underline{F}^{-1}\underline{B}\,{}_4a^* \,.$$

The matrix $\underline{B}^{-1}\underline{F}^{-1}\underline{B}$ is given by :

$$
\underline{B}^{-1}\underline{F}^{-1}\underline{B} \;=\; \left(\begin{array}{c|c} B^{-1} & 0 \\ \hline {}^{\mathrm{t}}\xi & \xi_\perp \end{array}\right) \left(\begin{array}{c|c} F^{-1} & 0 \\ \hline 0 & \pm 1 \end{array}\right) \left(\begin{array}{c|c} B & 0 \\ \hline -\frac{{}^{\mathrm{t}}\xi\,B}{\xi_\perp} & \frac{1}{\xi_\perp} \end{array}\right) \;=
$$

$$
=\; \left(\begin{array}{c|c} B^{-1}F^{-1}B & 0 \\ \hline {}^{\mathrm{t}}\xi\,(F^{-1} \mp I_3)\,B & \pm 1 \end{array}\right) \;. \qquad (1.2.19)
$$

$v'^{(4)}$ can be expressed either in terms of ${}_4a^*$, in which case $\underline{B}^{-1}\underline{F}^{-1}\underline{B}$ acts on $\ell^{(4)}$:

$$
{}^{\mathrm{t}}\ell^{(4)} \underline{B}^{-1}\underline{F}^{-1}\underline{B} \;=\; \left(\begin{array}{c|c} {}^{\mathrm{t}}\ell & m \end{array}\right) \left(\begin{array}{c|c} B^{-1}F^{-1}B & 0 \\ \hline {}^{\mathrm{t}}\xi\,(F^{-1} \mp I_3)\,B & \pm 1 \end{array}\right) \;=
$$

$$
=\; \left(\begin{array}{c|c} {}^{\mathrm{t}}\ell\,B^{-1}F^{-1}B + m\,{}^{\mathrm{t}}\xi\,(F^{-1} \mp I_3)\,B & \pm m \end{array}\right) \qquad (1.2.20)
$$

or in terms of new basis vectors :

$$
\underline{B}^{-1}\underline{F}^{-1}\underline{B}\,{}_4a^* \;=\; \left(\begin{array}{c|c} B^{-1}F^{-1}B & 0 \\ \hline {}^{\mathrm{t}}\xi\,(F^{-1} \mp I_3)\,B & \pm 1 \end{array}\right) \left(\begin{array}{c} a^* \\ X \end{array}\right) \;=
$$

$$
=\; \left(\begin{array}{c} B^{-1}F^{-1}B\,a^* \\ {}^{\mathrm{t}}\xi\,(F^{-1} \mp I_3)\,B\,a^* \pm X \end{array}\right) \,, \qquad (1.2.21)
$$

in which case the components $\ell^{(4)}$ remain the same. Expression 1.2.20 shows that the three first integer components ℓ are transformed into components containing ℓ and m, which is unsuitable as the first three components are always associated with main spots.

$v'^{(4)}$ must then be seen as a vector with the same components as $v^{(4)}$, but expressed in another basis, given by relation 1.2.21. This relation is particularly interesting because it shows that the transformation of the vector X is not linear, a type of translation is present. This phenomenon is due to the difference in the nature of the indices $\ell \in \mathbb{Z}^3$ and $m \in \mathbb{Z}$; ℓ corresponds to the integer column-vector with respect to $\{a^{*1}; a^{*2}; a^{*3}\}$ starting at a fixed point, called *origin* of the reciprocal space, whereas m expresses the position of the m-th satellite spot with respect to its associated main spot. The localisation of the satellite spots is then ambiguous : the only index m of a satellite spot does not specify its association with a main spot; hence the presence of this additive translation part ${}^t\xi\,(F^{-1} \mp I_3)\,B\,a^*$ in order to assure the affiliation to the right main spot.

As both vectors $v^{(4)}$ and $v'^{(4)}$ are elements of $\Lambda^{*(4)}$, their components with respect to the basis $\{a^{*1}; a^{*2}; a^{*3}; X\}$ must be integer. This implies that $B^{-1}F^{-1}B$ as well as ${}^t\xi\,(F^{-1}\mp I_3)\,B$, therefore $\underline{B^{-1}\underline{F^{-1}}\underline{B}}$, must contain only integer numbers. For $B^{-1}F^{-1}B$, this is of course the case, as F^{-1} is a matrix leaving the diffraction pattern invariant. Regarding ${}^t\xi\,(F^{-1}\mp I_3)\,B$, it is integer only if ξ satisfies some conditions. Decomposing ξ in a rational and an irrational part, $\xi = {}_r\xi + {}_i\xi$, and inserting these in ${}^t\xi\,(F^{-1}\mp I_3)\,B$, we obtain :

$$ {}^t\xi\,(F^{-1}\mp I_3)\,B = {}^t({}_r\xi)\,(F^{-1}\mp I_3)\,B + {}^t({}_i\xi)\,(F^{-1}\mp I_3)\,B \; . \qquad (1.2.22) $$

In order to obtain an integer expression, ${}^t({}_i\xi)\,(F^{-1}\mp I_3)\,B$ must be equal to zero, otherwise it would be irrational, hence non-integer. Thus, we have the condition :

$$ {}^t({}_i\xi)\,F^{-1}B = \pm{}^t({}_i\xi) \quad \Leftrightarrow \quad {}^tB\,F\,{}_i\xi = \pm{}_i\xi \; , \qquad (1.2.23) $$

which implies :

$$ {}^t\xi\,(F^{-1}\mp I_3)\,B = {}^t({}_r\xi)\,(F^{-1}\mp I_3)\,B \quad \Leftrightarrow $$

$$ \Leftrightarrow \quad {}^tB\,(F\mp I_3)\,\xi = {}^tB\,(F\mp I_3)\,{}_r\xi \; . \qquad (1.2.24) $$

All the previous considerations show that symmetry operations of modulated crystals extended to four dimensions are strongly correlated to those of the corresponding non-distorted three-dimensional structure. A distinction between general four-dimensional crystals and three-dimensional modulated structures extended to four dimensions must be considered. To note the difference, these latter are called $(3 + 1)$-dimensional structures; the set of all symmetry operation of such a structure is called a $(3+1)$-*dimensional superspace group*, whereas the set of all symmetry operations of a general four-dimensional crystal is called a *four-dimensional space group*. Both are groups in the mathematical meaning and a $(3 + 1)$-dimensional superspace group is always a subgroup of a four-dimensional space group. As superspace symmetry operations are closely connected to space group operations, the three dimensional space group appears in the nomenclature of superspace groups. Two different notations exist : *one-line* and *two-line symbols*.

The one-line symbol is composed of three parts; the first part gives the symbol of the three-dimensional space group of the corresponding non-distorted three-dimensional crystal; the second part contains three greek letters in parentheses $(\alpha\beta\gamma)$ that correspond to the components of the modulation vector with respect to the reciprocal basis $\{a^{*1}; a^{*2}; a^{*3}\}$; the third part, consisting of one, two or three of the symbols $\{0, s, t, q \text{ or } h\}$, indicates the *intrinsic translation part* of the symmetry operations in the fourth dimension. By a suitable choice of the origin, the translation part of any three-dimensional space group operation can be reduced to its *intrinsic part* (see chapter 4). In the same way, the translation part $s^{(4)}$ of a superspace symmetry operation can be reduced to its intrinsic part. As the matrix part F of a three-dimensional symmetry operation can be only of order $N \in \{1; 2; 3; 4; 6\}$, that is $F^N = I_3$, so it is for $\underline{F}$ given in expression 1.2.16. This implies that the fourth component of the intrinsic translation can only be equal to 0, $\frac{1}{2}$, $\pm\frac{1}{3}$, $\pm\frac{1}{4}$ or $\pm\frac{1}{6}$, modulo integers, with respect to the direct lattice basis $\{_4a_1; {}_4a_2; {}_4a_3; {}_4a_4\}$. To each of this values, a letter or a zero is associated, as follows :

$$
\begin{array}{ccccc}
0 & \frac{1}{2} & \pm\frac{1}{3} & \pm\frac{1}{4} & \pm\frac{1}{6} \\
0 & s & t & q & h
\end{array}
\quad .
$$

In the case where the component $(4; 4)$ of $\underline{F}$ is equal to -1, the fourth component of the intrinsic translation is equal to zero. In the third part of the one-line superspace group nomenclature, the number of letters or/and zeros is equal to the number of signs appearing after the capital letter in the space group symbol. Each of these signs designates a generator of the group other than a pure translation, that is a symmetry operation generating all the others of the group, except possibly the pure translations. With each of this operation is associated a superspace operation composed of a matrix part and a translation part that can be reduced to the intrinsic part in which appears the intrinsic part in the fourth dimension. To illustrate our purpose, we consider the superspace group of sodium carbonate studied by Pieter de Wolff :

$$C\,2/m(\alpha 0\gamma)0s \ .$$

- The first part, $C\,2/m$, indicates that the crystal system of the corresponding non-distorted structure is monoclinic; if $a_1 \doteq a$, $a_2 \doteq b$ and $a_3 \doteq c$ are three vectors generating a unit cell of the structure, two angles between these vectors are equal to $\frac{\pi}{2}$. By convention, it is the b vector which is normal to the plane spanned by a and c. The letter C, refers to the Bravais lattice and indicates a centring in the plane spanned by a and b. $2/m$ stands for a rotation of angle π around the vector b and a mirror operation the mirror plane of which is normal to b.

- The second part, $(\alpha 0\gamma)$, corresponds to the components of the wave vector (or modulation vector) ξ given with respect to the reciprocal basis vectors $a^{*1} \doteq a^*$, $a^{*2} \doteq b^*$, $a^{*3} \doteq c^*$ defined by the relation $a^{*i} \cdot a_j = \delta^i{}_j$. We notice that ξ lies in the plane spanned by a^{*1} and a^{*3}, that is by a and c.

- The third part, 0s, gives information about the fourth component of the intrinsic translation of the superspace symmetry operation associated with each generator

of the three-dimensional space group. With the rotation of angle π is associated the intrinsic translation 0 in the fourth dimension, while a value $\frac{1}{2}$ corresponds to the mirror operation m.

The value of the intrinsic translation in the fourth dimension can be partially deduced from the action of the matrix part F of a symmetry operation on the wave vector ξ. In order that main spots be transformed into main spots and satellite spots into satellite spots, ξ can be only transformed into $\pm\xi$:

$$F\,\xi = \pm\xi + {}^{t}(B^{-1})\,\ell\ , \qquad \ell \in \mathbb{Z}^3\ . \tag{1.2.25}$$

This relation seems to be incorrect, as a linear transformation cannot generate a translation. Nevertheless, the additional vector ${}^{t}(B^{-1})\,\ell$ must be present in order to satisfy equation 1.2.21 and its consequences concerning the index m. If F corresponds to the rotation of angle π about the b (or equivalently b^*), then $F\,\xi = -\xi$, implying that the intrinsic translation in the fourth dimension is equal to zero. If F corresponds to the mirror operation, then $F\,\xi = \xi$ and the intrinsic translation in the fourth dimension is not necessarily equal to zero; note that it cannot be equal to $\pm\frac{1}{3}$, $\pm\frac{1}{4}$ or $\pm\frac{1}{6}$, as the order of the mirror operation is equal to two.

Note that equation 1.2.25 imposes restrictions on the vector ξ. For instance, if F represents a rotation of an angle smaller than π about a certain axis, the equation $F\,\xi = \pm\xi$ is satisfied only if ξ is parallel to the rotation axis. This implies that the modulation can be only along the main axis (that is the axis corresponding to the rotation of highest order) in the trigonal, tetragonal or hexagonal crystal systems; the component of ξ would be (00γ) in all these cases. However, as the transformation of ξ through F is always defined within a vector ${}^{t}(B^{-1})\,\ell$, the first two components may be fractional numbers different from zero. All possible rational parts of a modulation wave vector are given in the following table :

P	(000)	R	$(\frac{1}{3}\frac{1}{3}0)$		
A	$(\frac{1}{2}00)$	B	$(0\frac{1}{2}0)$	C	$(00\frac{1}{2})$
L	(100)	M	(010)	N	(001)
U	$(\frac{1}{2}\frac{1}{2}0)$	V	$(\frac{1}{2}0\frac{1}{2})$	W	$(0\frac{1}{2}\frac{1}{2})$

As the components of the vector ξ are given with respect to a reciprocal basis, the direct basis of which is not necessarily primitive, integer numbers may also appear in the rational part. Contrary to the one-line symbol, the two-line symbol of superspace group contains only the information about the rational part of the modulation wave vector. In order to achieve a more compact notation, a capital letter is assigned to each possibility, as it is shown in the table above. This letter is followed by the space group symbol of the corresponding non-modulated structure in the upper line, and by the intrinsic translation in the fourth dimension associated to each generator of the space group in the bottom line. In the case of an inversion of ξ, the inversion symbol $\bar{1}$ is

indicated instead of the zero value of the intrinsic translation in the fourth dimension. For instance, the two-line superspace group symbol of sodium carbonate is :

$$P^{C\,2/m}_{\ \bar{1}\ \ s}\ .$$

The letter P indicates that all components of the rational part of the modulation wave vector are equal to zero; in the bottom line, we notice the intrinsic translations in the fourth dimension previously discussed in the case of the one-line superspace group symbol.

The number of modulations in a crystal is not limited to one. Structures containing two or even three modulations are not so rare. For more than one modulations, the modulation wave vectors have different orientations, but not necessarily different norms. Again, the characteristics of these vectors, as well as the connection between them, is laid down by the three-dimensional symmetry of the corresponding non-distorted structure. All concepts and derivations previously done for the case of one modulation, can easily be generalised to two or three modulations. Note that the number of modulations cannot be higher than three, as a modulation is by definition a periodic deformation, and the space in which a crystal exists is of dimension three.

Since the resolution and refinement of sodium carbonate by Pieter de Wolff and coworkers in 1974, a substantial number of modulated crystals, inorganic or, more recently organic, has been discovered and solved (see for instance the articles [BBD^{+}01, SC04]). Many different shapes of modulations have been considered, smooth as well as only piecewise smooth functions, of *crenel* or *saw-tooth* shape. However, it is not really clear to what extent the superspace formalism, in particular superspace symmetry operations, is used in the resolution of a modulated structure. Indeed, the procedure consists first in solving the average (non-modulated) structure; then, each atom in this three dimensional structure is considered as a periodic line, or surface or volume, in a four-, or five- or six-dimensional space, which is written as a Fourier series; one tries to refine the modulated structure by considering only the fundamental term in the series; if this does not work, higher order terms are considered. Thus, the superspace symmetry operations play a role in the refinement, but not in the resolution of the average structure. In the *charge flipping* algorithm, the procedure is different : a modulated structure is considered and solved as a $(3+d)$-dimensional structure, $d = 1, 2, 3$; from the beginning, a three-dimensional modulated crystal is seen as a higher-dimensional structure, as a crystal in the superspace. However, the superspace symmetry operations are not of prime importance, as the structure is solved without taking advantage of its symmetry [Pal04, PDGB06].

It must be borne in mind that in the expression of the electron density of a modulated structure extended to four dimensions, the fourth coordinate has a different status compared to the first three. This is well expressed by the fact that the matrix part of a superspace symmetry operation never acts as a 4×4 block in the electron density of a $(3+1)$-dimensional structure, but as a 3×3 and a 1×1 blocks. The structure factor, *i.e.* the Fourier transform of the electron density, can never be simplified as in the case of a three-dimensional structure. One can then wonder if the superspace formalism was not invented just for didactic reasons, for crystallographer-brains conditioned by the fact that a symmetry operation must be written as a matrix and translation parts...

Notice that the superspace formalism is not the only model that has been proposed for the description of the symmetry of modulated structures. In 1983, J. M. Perez-Mato and coworkers showed that superspace groups can be introduced through the invariance properties of the so-called *Landau free-energy expansion*, avoiding any reference to the diffraction pattern [PMMT84]. Twelve years later, J. Dräger and N. D. Mermin [DM96] suggested a model within which the symmetry of modulated crystals appears in the *gauge function* expressing the indistinguishability of the Fourier coefficients of the electron density of a structure. If both do not require a higher-dimensional space for the description of the symmetry of modulated structures, they nevertheless do not offer methods for determining such structures.

1.3 Motivation for Using Differential Geometry

Differential geometry is a mathematical discipline used in different physical domains, as for instance analytical mechanics or relativity, but rarely in crystallography. In fact, as long as a situation or a phenomenon may be described with respect to a *cartesian coordinate system*, that is the usual coordinate system of the Euclidean space, differential geometry is avoided. This latter only appears when curves, curved surfaces or spaces are considered and when a description with respect to a *cartesian coordinate system* becomes too cumbersome or problematic.

Such a complication has, however, appeared and taken some importance for several years in the frame of the study of a possible connection between space groups and the symmetry of tilings in the two-dimensional hyperbolic space, the latter being a typical example of a curved space, for which a cartesian coordinate system is not adapted at all. S. T. Hyde and coworkers have shown that two-dimensional curved surfaces in the three-dimensional Euclidean space possessing three-dimensional periodicity can be considered as a three-dimensional periodic repetition of a polygon, a tile of the two-dimensional hyperbolic space, by an appropriate zipping of its sides [HLM$^+$03, HFRR06, RRH09]. The symmetry of the surface in three-dimensions can then be expressed in terms of the symmetry of a tiling in the two-dimensional hyperbolic space. Thus, space groups could be represented as two-dimensional hyperbolic isometry groups, offering a substantial advantage in the case of trigonal, tetragonal, hexagonal and in particular cubic groups, which are particularly difficult to illustrate with figures.

As seen in the previous subsection, a crystal is an object existing in our three-dimensional space which can be seen as a three-dimensional point space endowed with a *cartesian coordinate system*, that is three axes generated by an orthonormal vector basis of the associated vector space. Any atom of any crystal, be it modulated or not, can be located with respect to these three axes. Such a coordinate system is, however, not systematically used for describing the geometry and symmetry of crystals, even for non-modulated ones; crystallographers do not hesitate and even prefer to introduce other coordinate systems, still composed of three straight line axes, but generated by a vector basis particularly adapted to the shape of the unit cell generating the crystal. One can then wonder why a curved coordinate system is not introduced for modulated structures; why have crystallographers stopped halfway? It is right that a formalism
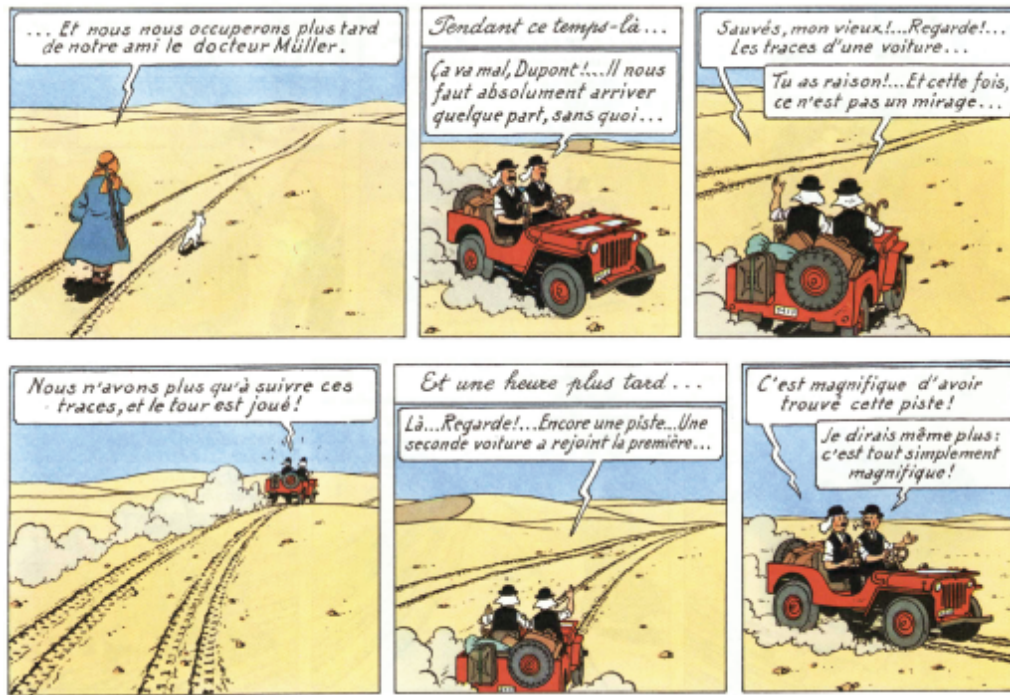
Figure 1.1: In the strip cartoon *Tintin au pays de l'or noir*, the Dupondt policemen, without any landmark, are driving around in circles in the desert.

involving a curved coordinate system, in which vectors are replaced by curves, requires some efforts. Nevertheless, once this effort has been provided, life becomes beautiful because one is no longer the slave of a predefined framework.

One is forced to notice that straight lines seldom appear in real life. Who can pretend to walk from a point to another in a straight line? Most of the time, one does not follow a straight line, and realises it only sometimes. Examples are multiple : when crossing the street in a (pretended) straight line, one first goes down from the sidewalk to the street and then goes up to another sidewalk; when climbing a mountain, one does not in general walk along a straight line from the starting to the end points, the way is much longer, adapted to the shape of the mountain and to human possibilities. These two examples involve the particular geometry of the considered surface (the street or the mountain). Notwithstanding this, many other situations exist where one could, but because of constraints, does not walk in a straight line : who has not made a detour in order to cross the way of a beautiful young lady or a charming prince? Who has not made a detour in order to pass near a pub where they serve lovely stout or other kinds of tasty beers? More seriously, who could pretend to be better than the Dupondt policemen (see figure 1.1) and say that he or she would be walking or driving in a straight line in the desert or to a particular place without a landmark?

If straight lines are rare in concrete life, the physical world concedes them more importance, without privileging them. Differential geometry effectively treats *curved* spaces, while also including *flat* spaces as a particular case. It is therefore a large enough framework for geometrically describing physical situations or phenomena. The effort required to be familiar with the formalism is substantial, but not at all in vain!

Chapter 2

Representation of a Structure in a Manifold

The appropriate tool for describing the concept of repetition of a brick in three (or $n \in \mathbb{N} \smallsetminus \{0\}$) dimensions is the so-called *group of translations* and its action on the points of a *metric space*.

When the metric space corresponds to the Euclidean space (that is the so-called point space), the action of a translation on a point consists in adding one real number to each of its coordinates. If this holds in the case of the Euclidean space, it certainly does not for a general metric space, for instance a curved surface or a curved space. Thus, in order to have a definition of the concept of translation taking into account the geometry of the considered space, a more general framework is required; the point space has to be replaced by the concept of manifold and the translation group must be treated as a Lie group.

In this way, a unified description of crystals, whether modulated or not, may be obtained. Moreover, new definitions of *space* and *point group operations* can be given, without resorting to additional dimensions in the case of modulated structures.

2.1   Riemannian Manifolds

The notion of *manifold* is a generalisation of objects like curves and surfaces the geometrical properties of which have been abundantly treated by Gauß, and later by Riemann. The main concepts from manifold theory are presented in the next subsection. A more advanced treatment may be found in the monographs by Barrett O'Neill [O'N83] and Norbert Straumann [Str84].

2.1.1   Manifold and Tangent Spaces

A *manifold M* of dimension n is a Hausdorff (separated, topological) space such that for all point $p \in M$, there exists a homeomorphism φ (see appendix A) between an open neighbourhood $\mathcal{U} \subset M$ containing p and an open neighbourhood $\mathcal{U}' \subset \mathbb{R}^n$. The couple $(\mathcal{U}; \varphi)$ is called *coordinate system*, and the couple $(\mathcal{U}'; \varphi^{-1})$ a (local) *parameterisation*

of M. If $(\mathcal{U}_1;\ \varphi_1)$ and $(\mathcal{U}_2;\ \varphi_2)$ are two different coordinate systems such that $\mathcal{U}_1 \cap \mathcal{U}_2 \neq \varnothing$, then

$$\varphi_2 \circ {\varphi_1}^{-1} : \varphi_1(\mathcal{U}_1 \cap \mathcal{U}_2) \longrightarrow \varphi_2(\mathcal{U}_1 \cap \mathcal{U}_2)$$

is called *change of coordinates.* If $\varphi_2 \circ {\varphi_1}^{-1}$ is of class C^∞ (the set of all functions which can be differentiated infinitely many times), we say that the change of coordinate is *smooth.* A family

$$\mathcal{A} = \{(\mathcal{U}_i;\ \varphi_i) \mid i \in I\}$$

of coordinate systems (where I is a countable ensemble) is called an *atlas* of M if $\bigcup_{i \in I} \mathcal{U}_i = M$. If all changes of coordinates are smooth, we say that the atlas is smooth and M is a smooth manifold.

As examples of manifolds, we can first mention the n-dimensional Euclidean space $\mathbb{R}^n$; the identity map $\varphi = (u^1;\ \dots;\ u^n)$ is a one-coordinate system atlas. The two-dimensional sphere $\mathcal{S}^2$ ($\subset \mathbb{R}^3$) is a two-dimensional manifold, which is usually parameterised with the latitude and longitude angles θ and φ respectively. Generally speaking, every surface in the three-dimensional Euclidean space (*e.g.* cylinder, torus, paraboloid) is a two-dimensional manifold.

Let $p \in M$ be a point in a smooth manifold M. Let $C_p^\infty(M)$ be the set of smooth functions in a neighbourhood containing p, and $C^\infty(M)$ the set of smooth functions in M. A *tangent vector v* to M at p is a map

$$\begin{aligned} v : C_p^\infty &\longrightarrow \quad \mathbb{R} \\ f &\longmapsto \quad v[f](p) \end{aligned}$$

such that for all $f_1, f_2 \in C_p^\infty(M)$ and $a, b \in \mathbb{R}$:

1. $v[a\, f_1 + b\, f_2] = a\, v[f_1] + b\, v[f_2]$ (linearity),

2. $v[f_1\, f_2] = v[f_1]\, f_2(p) + f_1(p)\, v[f_2]$ (Leibnitz' rule).

For each $p \in M$, the set of tangent vectors to M at p has the structure of a vector space. It is called *tangent space* of M at p and noted $\mathrm{T}_p M$. As an example of a tangent vector, we immediately think of a ship sailing on the sea. At any point p of the sea (on Earth's surface), her velocity vector is a tangent vector to our Earth at this point.

Let $(\mathcal{U};\ \varphi)$, $\varphi = (x^1;\ \dots;\ x^n)$, be a coordinate system of a manifold M at p, and $(u^1;\ \dots;\ u^n)$ the natural coordinate system in $\mathbb{R}^n$ (the identity map of $\mathbb{R}^n$); note that $u^i \circ \varphi = x^i$. For any function $f \in C^\infty(M)$, we define :

$$\left.\frac{\partial}{\partial x^i}\right|_p f = \frac{\partial f}{\partial x^i}(p) = \frac{\partial(f \circ \varphi^{-1})}{\partial u^i}\big(\varphi(p)\big) , \qquad 1 \leqslant i \leqslant n .$$

A calculation shows that $\partial_i\big|_p \doteq \left.\frac{\partial}{\partial x^i}\right|_p : C_p^\infty(M) \to \mathbb{R}$ is a tangent vector to M at p. One also shows that the set of derivatives $\big(\partial_1\big|_p ;\ \dots ;\ \partial_n\big|_p\big)$ forms a basis of the tangent space $\mathrm{T}_p M$ at p; this basis is called *canonical basis* of $\mathrm{T}_p M$. Thus any tangent vector $v \in \mathrm{T}_p M$ may be written as $v = \sum_{i=1}^n v^i\, \partial_i\big|_p$, where $v^i = v[x^i](p)$.

A *smooth curve* on a manifold M is a map $\gamma : I \to M$, where I is an open interval in $\mathbb{R}$. At each $t \in I$, we can consider its tangent vector, noted $\dot{\gamma}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\gamma(t)$, which acts on any function $f \in C^\infty_{\gamma(t)}(M)$ as :

$$\dot{\gamma}(t)[f] = \frac{\mathrm{d}(f \circ \gamma)(t)}{\mathrm{d}t} = \sum_{i=1}^n \frac{\mathrm{d}(x^i \circ \gamma)(t)}{\mathrm{d}t} \partial_i\big|_{\gamma(t)} f \ .$$

Note that $(x^1 \circ \gamma \, ; \, \ldots \, ; \, x^n \circ \gamma)$ is nothing else than the coordinate representation of γ.

It is interesting to notice that the tangent space to a manifold M at a point p can also be defined by considering the derivative at p of any smooth curve going through p. Indeed, let $\mathcal{C}_p(M)$ be the set of all curves $(I; \gamma)$ (or γ for short), such that $0 \in I$ and that $\gamma(0) = p$. The subset of $(I; \gamma)$ in which all curves have the same derivative at 0 form an equivalence class. Such a class is called *tangent vector* at p and is noted

$$\dot{\gamma}(0) = \frac{\mathrm{d}}{\mathrm{d}t}\gamma(t)\big|_{t=0} \quad .$$

Two curves $(I_1; \gamma_1), (I_2; \gamma_2) \in \mathcal{C}_p(M)$ have the same tangent vector at p if :

$$\frac{\mathrm{d}}{\mathrm{d}t}(f \circ \gamma_1)\big|_{t=0} = \frac{\mathrm{d}}{\mathrm{d}t}(f \circ \gamma_2)\big|_{t=0} \, , \quad \forall \, f \in C^\infty(M) \quad .$$

Since the derivative is a linear map, the set of all tangent vectors at p has the structure of a vector space; it is called *tangent space* at p and is noted $\mathrm{T}_p M$.

The set of all tangent vectors to a smooth manifold M has a vector *bundle* structure; it is called *tangent bundle* and is noted $\mathrm{T}M$. A vector v belongs to $\mathrm{T}M$ if and only if there exists a point $p \in M$ such that $v \in \mathrm{T}_p M$. Thus, $\mathrm{T}M$ may be written as $\mathrm{T}M = \bigcup_{p \in M} \mathrm{T}_p M$. A *vector field* on an open set $\mathcal{W} \subset M$ is a map $Y : \mathcal{W} \to \mathrm{T}M$ which assigns to each point $p \in M$ a tangent vector $Y_p \in \mathrm{T}_p M$. Y is *smooth* if it is smooth at any $p \in \mathcal{W}$. A simple example of a vector field on a manifold is given by the set of tangent vectors at each point of Earth turning about itself.

Let $(\mathcal{U}; \varphi)$, $\varphi = (x^1; \ldots; x^n)$, be a coordinate system of a manifold M. Then, for each $1 \leqslant i \leqslant n$, the map carrying any point $p \in \mathcal{U}$ into $\partial_i\big|_p$ is a vector field; it is smooth because $\partial_i f = \frac{\partial f}{\partial x^i}$, $f \in C^\infty$, is smooth. The vector fields $\partial_1; \ldots; \partial_n$ are called *coordinate vector fields* associated to the coordinate system $(\mathcal{U}; \varphi)$. As in the case of tangent vectors, any field $Y : \mathcal{U} \to \mathrm{T}M$ can be written as $Y = \sum_{i=1}^n y^i \, \partial_i$, where $y^i = Y[x^i]$.

2.1.2 Isometries on a Riemannian Manifold

A *metric tensor* g on a smooth manifold M is a symmetric, positive definite $(0; 2)$ (*i.e.* two times covariant) tensor field on M. In other words :

$$\begin{aligned} g : \mathrm{T}M \times \mathrm{T}M &\longrightarrow \mathbb{R} \\ (v; w) &\longmapsto g(v; w) \quad ; \end{aligned}$$

g associates each point $p \in M$ with a scalar product g_p in the tangent space $\mathrm{T}_p M$ at p. A smooth manifold M furnished with a metric tensor g is called a *Riemannian manifold* and is noted $(M; g)$.

Let $(\mathcal{U}; \varphi)$, $\varphi = (x^1; \ldots; x^n)$, be a coordinate system at a point $p \in M$ and $\partial_1, \ldots, \partial_n$ (where $\partial_i = \frac{\partial}{\partial x^i}$) the associated coordinate vector fields. The functions g_{ij} defined by :

$$g_{ij} = g(\partial_i; \partial_j) \quad , \quad 1 \leqslant i, j \leqslant n \ ,$$

are called *components of the metric tensor* g. For any two vector fields Y and Z, written as $Y = \sum_{i=1}^n y^i \, \partial_i$ and $Z = \sum_{j=1}^n z^j \, \partial_j$, we have :

$$g(Y; Z) \, = \, g\left(\sum_{i=1}^n y^i \, \partial_i \, ; \, \sum_{j=1}^n z^j \, \partial_j \right) \, = \, \sum_{i,j=1}^n y^i \, z^j \, g(\partial_i; \partial_j) \, = \, \sum_{i,j=1}^n y^i \, z^j \, g_{ij} \ .$$

Thanks to the metric tensor, the notions of length of curves on a manifold and angles between tangent vectors can be defined. Moreover, Riemannian manifolds can be seen as metric spaces. Indeed, in every connected manifold, we can define the distance between two points p and q as the length of the curve of minimal length belonging to the manifold and linking these two points. In many cases, especially when the manifold has no boundary, this curve is a *geodesic* (this last concept will be tackled later).

Let M and $\tilde{M}$ be two manifolds of dimension n and m respectively, $\mathcal{W} \subset M$ an open set and ϕ a smooth map from $\mathcal{W}$ to $\tilde{M}$. For any point $p \in \mathcal{W}$, the map

$$\mathrm{d}\phi_p : \mathrm{T}_p M \ \longrightarrow \ \mathrm{T}_{\phi(p)} \tilde{M}$$

given by :

$$\mathrm{d}\phi_p(v)[f]\big(\phi(p)\big) = v[f \circ \phi](p) \ , \qquad \forall \ v \in \mathrm{T}_p M \ \text{and} \ f \in C^\infty(\phi(\mathcal{W})) \ ,$$

is linear and is called *differential map* of ϕ at p. If $(\mathcal{U}; \varphi)$, $\varphi = (x^1; \ldots; x^n)$, is a coordinate system of M at p and $(\tilde{\mathcal{U}}; \tilde{\varphi})$, $\tilde{\varphi} = (\tilde{x}^1; \ldots; \tilde{x}^n)$, a coordinate system of $\tilde{M}$ at $\phi(p)$, then :

$$\mathrm{d}\phi_p\big(\partial_i\big|_p\big) = \sum_{j=1}^n \frac{\partial(\tilde{x}^j \circ \phi)}{\partial x^i}(p) \, \tilde{\partial}_j\big|_{\phi(p)} \ , \qquad 1 \leqslant i \leqslant n \ , \tag{2.1.1}$$

where $\partial_i\big|_p = \frac{\partial}{\partial x^i}\big|_p$ and $\tilde{\partial}_j\big|_{\phi(p)} = \frac{\partial}{\partial \tilde{x}^j}\big|_{\phi(p)}$. The matrix $\big(\frac{\partial(\tilde{x}^i \circ \phi)}{\partial x^j}\big)_{i,j=1}^n$ is called *jacobian matrix* of the change of coordinates.

Let us focus on the case where $\tilde{M} = M$. A map $\phi : M \to M$ is called *local isometry* if for all $p \in M$ and $v, w \in \mathrm{T}_p M$:

$$g\big(\mathrm{d}\phi_p(v); \mathrm{d}\phi_p(w)\big) = g(v; w) \quad ; \tag{2.1.2}$$

it is an *isometry* if it is also a diffeomorphism (see appendix A). The set of all isometries of M,

$$\mathrm{Isom}(M) = \ \{\phi : M \to M \mid \phi \text{ is an isometry}\}$$

has the structure of a group. It is called the *isometry group* of M.

Although this definition is specific to manifold theory, it is completely consistent with the common intuitive notion of isometry. Indeed, with this definition, lengths of curves and angles between two curves at their intersection remain unchanged under an isometry. To see that concretely, consider an isometry ϕ and two curves $(I_1; \gamma_1)$ and $(I_2; \gamma_2)$ which intersect at the point p. By the definition of the length of a curve, the length of γ_1 (for instance) is :

$$\ell_{\gamma_1} = \int_{t_1}^{t_2} \sqrt{g\big(\dot{\gamma}_1(t) \,;\, \dot{\gamma}_1(t)\big)} \ \mathrm{d}t \ ,$$

where t_1 and t_2 are the boundary points of the interval I_1. The length of the image curve $\phi \circ \gamma_1$ is :

$$\ell_{\phi(\gamma_1)} = \int_{t_1}^{t_2} \sqrt{g\Big(\mathrm{d}\phi_{\gamma_1(t)}\big(\dot{\gamma}_1(t)\big) \,;\, \mathrm{d}\phi_{\gamma_1(t)}\big(\dot{\gamma}_1(t)\big)\Big)} \ \mathrm{d}t \ .$$

Since

$$g\Big(\mathrm{d}\phi_{\gamma_1(t)}\big(\dot{\gamma}_1(t)\big) \,;\, \mathrm{d}\phi_{\gamma_1(t)}\big(\dot{\gamma}_1(t)\big)\Big) \ = g\big(\dot{\gamma}_1(t) \,;\, \dot{\gamma}_1(t)\big) \ ,$$

then the length $\ell_{\phi(\gamma_1)}$ is equal to the length ℓ_{γ_1}. If we consider the angle at the crossing point $p = \gamma_1(\tilde{t}) = \gamma_2(\tilde{t})$ of γ_1 and γ_2, which is given by :

$$\cos\theta = \frac{g\big(\dot{\gamma}_1(\tilde{t}) \,;\, \dot{\gamma}_2(\tilde{t})\big)}{\sqrt{g\big(\dot{\gamma}_1(\tilde{t}) \,;\, \dot{\gamma}_1(\tilde{t})\big) g\big(\dot{\gamma}_2(\tilde{t}) \,;\, \dot{\gamma}_2(\tilde{t})\big)}} \quad ,$$

we see that it is equal to the angle at the crossing point of the images curves $\phi(\gamma_1)$ and $\phi(\gamma_2)$, since :

$$\cos\theta \ = \ \frac{g\Big(\mathrm{d}\phi_{\phi(\gamma_1(\tilde{t}))}\big(\dot{\gamma}_1(\tilde{t})\big) \,;\, \mathrm{d}\phi_{\phi(\gamma_2(\tilde{t}))}\big(\dot{\gamma}_2(\tilde{t})\big)\Big)}{\sqrt{g\Big(\mathrm{d}\phi_{\phi(\gamma_1(\tilde{t}))}\big(\dot{\gamma}_1(\tilde{t})\big) \,;\, \mathrm{d}\phi_{\phi(\gamma_1(\tilde{t}))}\big(\dot{\gamma}_1(\tilde{t})\big)\Big) g\Big(\mathrm{d}\phi_{\phi(\gamma_2(\tilde{t}))}\big(\dot{\gamma}_2(\tilde{t})\big) \,;\, \mathrm{d}\phi_{\phi(\gamma_2(\tilde{t}))}\big(\dot{\gamma}_2(\tilde{t})\big)\Big)}} =$$

$$= \ \frac{g\big(\dot{\gamma}_1(\tilde{t}) \,;\, \dot{\gamma}_2(\tilde{t})\big)}{\sqrt{g\big(\dot{\gamma}_1(\tilde{t}) \,;\, \dot{\gamma}_1(\tilde{t})\big) g\big(\dot{\gamma}_2(\tilde{t}) \,;\, \dot{\gamma}_2(\tilde{t})\big)}}$$

The differential map at a point p of an isometry ϕ acts on vectors $\partial_i\big|_p$, $1 \leqslant i \leqslant n$, as follows (see expression 2.1.1) :

$$\mathrm{d}\phi_p\big(\partial_i\big|_p\big) = \sum_{j=1}^{n} \frac{\partial x'^j}{\partial x^i}(p) \, \partial_j\big|_{\phi(p)} \quad , \tag{2.1.3}$$

where $x'^j = x^j \circ \phi$, $1 \leqslant j \leqslant n$. If we use this expression in equation 2.1.2, in the case where $v = \partial_i\big|_p$ and $w = \partial_j\big|_p$, we obtain :

$$g\Big(\mathrm{d}\phi_p\big(\partial_i\big|_p\big); \mathrm{d}\phi_p\big(\partial_j\big|_p\big)\Big) \ = \ g\big(\partial_i\big|_p; \partial_j\big|_p\big) \quad \Leftrightarrow$$

$$g\left(\sum_{k=1}^{n} \frac{\partial x'^k}{\partial x^i}(p) \, \partial_k\big|_{\phi(p)} \,;\, \sum_{l=1}^{n} \frac{\partial x'^l}{\partial x^j}(p) \, \partial_l\big|_{\phi(p)}\right) \ = \ g\big(\partial_i\big|_p; \partial_j\big|_p\big) \ .$$

As g is a bilinear form, this expression can be rearranged as :

$$g\left(\sum_{k=1}^{n} \frac{\partial x'^k}{\partial x^i}(p)\, \partial_k\big|_{\phi(p)} \;;\; \sum_{l=1}^{n} \frac{\partial x'^l}{\partial x^j}(p)\, \partial_l\big|_{\phi(p)}\right) = \sum_{k,l=1}^{n} \frac{\partial x'^k}{\partial x^i}(p)\, \frac{\partial x'^l}{\partial x^j}(p)\, g\left(\partial_k\big|_{\phi(p)};\, \partial_l\big|_{\phi(p)}\right)$$

$$(2.1.4)$$

Thus, we finally have :

$$\sum_{k,l=1}^{n} \frac{\partial x'^k}{\partial x^i}(p)\, \frac{\partial x'^l}{\partial x^j}(p)\, g_{kl}\big(\phi(p)\big) = g_{ij}(p)\;. \tag{2.1.5}$$

This formula is very important, because it corresponds to the explicit condition for obtaining the general expression of any isometry on the considered manifold.

2.1.3   The Euclidean Manifold and its Isometry Group

The concept of *n-dimensional Euclidean manifold* can be defined in several different ways. One of the easiest ones is to say that it is a *flat* space, in the sense that it is a manifold which can be endowed with a one-coordinate system atlas with respect to which the metric tensor is represented by the identity matrix. Note that the existence of such a coordinate system does not necessarily imply its use. For instance, the three dimensional point space used by crystallographers, endowed with a *crystallographic coordinate system* $x = (x^1;\, \ldots;\, x^n)$, that is a system adapted to the geometry of the unit cell, is a Euclidean manifold; a coordinate system $u = (u^1;\, \ldots;\, u^n)$ in which the metric tensor is represented by the identity matrix is not necessarily used but it does exist : it is given by $x = B\,u$, for an appropriate matrix $B \in \mathrm{GL}_n(\mathbb{R})$. Typically, $\mathbb{R}^n$, endowed with the one coordinate system atlas $(\mathbb{R}^n;\, u)$, $u = (u^1;\, \ldots;\, u^n)$, in which the metric tensor is constant and represented by the identity matrix is Euclidean; this manifold will be called the *n-dimensional Euclidean manifold*.

Let ϕ be an isometry in the Euclidean manifold $\mathbb{R}^n$, endowed with the natural coordinate system $u = (u^1;\, \ldots;\, u^n)$. Equation 2.1.5 becomes in this case :

$$\sum_{k,l=1}^{n} \frac{\partial u'^k}{\partial u^i}(p)\, \frac{\partial u'^l}{\partial u^j}(p)\, \delta_{kl} = \delta_{ij}\;, \tag{2.1.6}$$

where $u'^k = u^k \circ \phi$, $1 \leqslant k \leqslant n$, and δ_{ij} is the *Kronecker symbol*. By taking the derivative of this expression with respect to u^m, we find :

$$\frac{\partial}{\partial u^m} \sum_{k,l=1}^{n} \frac{\partial u'^k}{\partial u^i}(p)\, \frac{\partial u'^l}{\partial u^j}(p)\, \delta_{kl} \;\; = \;\; \frac{\partial}{\partial u^m}\delta_{ij} \quad \Leftrightarrow$$

$$\Leftrightarrow \quad \sum_{k,l=1}^{n} \left(\frac{\partial^2 u'^k}{\partial u^m\, \partial u^i}(p)\, \frac{\partial u'^l}{\partial u^j}(p) + \frac{\partial u'^k}{\partial u^i}(p)\, \frac{\partial^2 u'^l}{\partial u^m\, \partial u^j}(p) \right) \delta_{kl} \;\; = \;\; 0\;. \tag{2.1.7}$$

Cyclic permutation of indices i, j and m yields :

$$\sum_{k,l=1}^{n} \left(\frac{\partial^2 u'^k}{\partial u^i \, \partial u^m}(p) \, \frac{\partial u'^l}{\partial u^j}(p) + \frac{\partial u'^k}{\partial u^m}(p) \, \frac{\partial^2 u'^l}{\partial u^i \, \partial u^j}(p) \right) \delta_{kl} \;\; = \;\; 0 \qquad (2.1.8)$$

$$\sum_{k,l=1}^{n} \left(\frac{\partial^2 u'^k}{\partial u^j \, \partial u^i}(p) \, \frac{\partial u'^l}{\partial u^m}(p) + \frac{\partial u'^k}{\partial u^i}(p) \, \frac{\partial^2 u'^l}{\partial u^j \, \partial u^m}(p) \right) \delta_{kl} \;\; = \;\; 0 \; . \qquad (2.1.9)$$

Adding expression 2.1.8 to expression 2.1.7 and subtracting relation 2.1.9, we find :

$$\sum_{k,l=1}^{n} \frac{\partial^2 u'^k}{\partial u^m \, \partial u^i}(p) \, \frac{\partial u'^l}{\partial u^j}(p) \, \delta_{kl} = 0 \; .$$

Multiplying this last equation by $\frac{\partial u^j}{\partial u'^r}$ and summing over j, we arrive at :

$$\frac{\partial^2 u'^r}{\partial u^i \, \partial u^m}(p) = 0 \; . \qquad (2.1.10)$$

This expression holds for all $1 \leqslant i, m, r \leqslant n$ and for each p. An integration gives :

$$f^r_{\;i} \doteq \frac{\partial u'^r}{\partial u^i} = \text{constant} \; ; \qquad (2.1.11)$$

After a second integration, we finally obtain :

$$u^r \circ \phi = u'^r = \sum_{i=1}^{n} f^r_{\;i} \, u^i + s^r \; , \qquad (2.1.12)$$

where s^r is a constant and $f^r_{\;i}$ is the component $(r; i)$ of a constant matrix F. Equation 2.1.6, which can be written in matrix notation :

$$^{\mathrm{t}}F \, F = I_n \; , \qquad (2.1.13)$$

shows that F is an orthogonal matrix. In another coordinate system $x = (x^1; \ldots; x^n)$, defined by $x = B \, u$, $B \in \mathrm{GL}_n(\mathbb{R})$, the matrix notation of equation 2.1.6 becomes :

$$^{\mathrm{t}}F \, G \, F = G \; , \qquad (2.1.14)$$

where G is the matrix representing the metric tensor in the coordinate system x; F would still be a constant matrix of determinant ± 1, however not orthogonal any more. In matrix notation, equation 2.1.12 is :

$$u' = F \, u + s \; , \qquad (2.1.15)$$

where $s \in \mathbb{R}^n$ is a constant. F and s are called the *matrix part* and the *translation part*, respectively. The set of all Euclidean isometries is called *Euclidean isometry group.*

The calculation presented here is not new at all; it can be found in any book treating differential geometry [O'N83], or relativity for instance [Das93]. It is, however, not mentioned in any book of crystallography. In excellent texts, such as those written by H. Wondratschek [Won02], D. Schwarzenbach and G. Chapuis [SC06] or P. Engel [Eng86], relation 2.1.15 is more or less presented as an axiom, whereas it is in fact the consequence of the definition of the n-dimensional Euclidean manifold.

2.2   Generation of a Lattice of Translation

The set of all Euclidean isometries, the matrix part of which is the identity matrix I_n corresponds to the translations in the Euclidean manifold. It has a group structure and is called *translation group*. Its study is primordial for understanding the notion of *periodicity* in a crystal structure.

2.2.1   The Translation group as a Lie Group

Relation 2.1.15 is often represented in a so called augmented form, where the matrix and translation parts are combined in one matrix of larger size :

$$
\begin{pmatrix} u'^1 \\ \vdots \\ u'^n \\ \hline 1 \end{pmatrix} = \left(\begin{array}{ccc|c} f^1_{\ 1} & \cdots & f^1_{\ n} & s^1 \\ \vdots & \ddots & \vdots & \vdots \\ f^n_{\ 1} & \cdots & f^n_{\ n} & s^n \\ \hline 0 & \cdots & 0 & 1 \end{array} \right) \begin{pmatrix} u^1 \\ \vdots \\ u^n \\ \hline 1 \end{pmatrix} .
$$

It is very practical but it presents the disadvantage that vectors have an additional component which does not have a physical meaning. Another, very elegant, way to combine the matrix and translation parts, without adding a dimension, consists in using the derivative technique; equation 2.1.12 can be written as :

$$
u'^i = \sum_{j=1}^n f^i_{\ j}\, u^j + s^i = \sum_{j=1}^n (f^i_{\ j}\, u^j + s^i\, \partial_i\, u^j) = \sum_{j=1}^n (f^i_{\ j} + s^i\, \partial_i)\, u^j .
$$

In matrix notation :

$$
\begin{pmatrix} u'^1 \\ \vdots \\ u'^n \end{pmatrix} = \left[\begin{pmatrix} f^1_{\ 1} & \cdots & f^1_{\ n} \\ \vdots & \ddots & \vdots \\ f^n_{\ 1} & \cdots & f^n_{\ n} \end{pmatrix} + \begin{pmatrix} s^1\, \partial_1 & & 0 \\ & \ddots & \\ 0 & & s^n\, \partial_n \end{pmatrix} \right] \begin{pmatrix} u^1 \\ \vdots \\ u^n \end{pmatrix}
$$

The expression in the brackets corresponds to an $n \times n$ matrix made up of the sum of the matrix F and another one, called S, describing the translation part. The translation part has then be absorbed, so that an isometric transformation in the Euclidean manifold can be written as :

$$
u' = \bar{F}\, u , \tag{2.2.1}
$$

where $\bar{F} \doteq F + S$.

In the case where $F = I_n$, the isometry corresponds to a *pure translation*; it is represented by the matrix $\bar{S} \doteq I_n + S$. The set of all pure translations is noted $\mathrm{Trans}(\mathbb{R}^n)$. Besides the fact that it is a group, it has also a manifold structure. Indeed, through the trivial parameterisation :

$$
(s^1; \ldots; s^n) \longmapsto \begin{pmatrix} 1 + s^1\, \partial_1 & & 0 \\ & \ddots & \\ 0 & & 1 + s^n\, \partial_n \end{pmatrix} ,
$$

it can be identified to the manifold $\mathbb{R}^n$. The translation group is then a *Lie group*. According to appendix B, to each Lie group is associated a Lie algebra, which mostly corresponds to the tangent space of the group at the origin of the coordinate system. The power of Lie theory is that the properties of Lie groups can be obtained by studying their associated algebra or, equivalently, their tangent space at the origin. In the case of the translations group, its Lie algebra is obtained by calculating the derivative of the matrix $\bar{S}$ with respect to s^i and taking its value at $s = 0$ (that is at $s = (s^1; \ldots; s^n) = (0; \ldots; 0)$) :

$$\left. \frac{\partial \bar{S}}{\partial s^i} \right|_{s=0} \doteq W_i \, , \tag{2.2.2}$$

with :

$$W_i = \begin{pmatrix} 0 & & & & \mathbf{0} \\ & \ddots & & & \\ & & \partial_i & & \\ & & & \ddots & \\ \mathbf{0} & & & & 0 \end{pmatrix} . \tag{2.2.3}$$

According to manifold theory, W_i is a tangent vector of $\mathrm{Trans}(\mathbb{R}^n)$ at the origin and the set of matrices $\{W_i \mid 1 \leqslant i \leqslant n\}$ constitutes a basis of the tangent space of $\mathrm{Trans}(\mathbb{R}^n)$ at the origin. This latter, which has a vector space structure, is noted $\mathfrak{trans}(\mathbb{R}^n)$ and the basis vectors $W_1, \ldots, W_n$ are called canonical basis vectors of $\mathfrak{trans}(\mathbb{R}^n)$. Any vector of $\mathfrak{trans}(\mathbb{R}^n)$ can be written as a linear combination of these canonical basis vectors.

As mentioned in appendix B, we can think of the Lie algebra $\mathfrak{g}$ of a Lie group $\mathcal{G}$ as the tangent space of this latter at the origin, as they are isomorphic. As its name indicates, the Lie algebra (tangent space at the origin) $\mathfrak{g}$ of a Lie group $\mathcal{G}$ is not only a vector space but an algebra. Indeed, beside the addition operation, the vector space is furnished with a bilinear function $\mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, called *Lie bracket operation*, which has *skew-symmetry* property and which satisfy the *Jacobi identity*. In the case of invertible matrices, the bracket operation is simply the commutator of two matrices :

$$[A \, ; \, B] = A\,B - B\,A \in \mathrm{GL}_n(\mathbb{R}) \quad , \quad \forall \, A, B \in \mathrm{GL}_n(\mathbb{R}) \, .$$

In the special case of translations, $\mathfrak{trans}(\mathbb{R}^n)$ is also closed under the commutator operation; indeed, for any two matrices W_i and W_j, $1 \leqslant i, j \leqslant n$, of the canonical basis of $\mathfrak{trans}(\mathbb{R}^n)$, we have :

$$[W_i \, ; \, W_j] = 0_n \, \in \mathfrak{trans}(\mathbb{R}^n) \, . \tag{2.2.4}$$

$\mathfrak{trans}(\mathbb{R}^n)$ is then an algebra.

The connection between a Lie algebra and its corresponding Lie group is given by the exponential map (see appendix B) : each element of the group can be written as the exponential of an element of the associated Lie algebra. In the case of invertible matrices, the exponential map is the usual exponential function given by its power series. Extending this result to the translations group, we obtain, in the case of the vector $s^i\,W_i$, where W_i is a canonical vector of $\mathfrak{trans}(\mathbb{R}^n)$ and $s^i \in \mathbb{R}$:

$$\exp(s^i\,W_i) = \sum_{k=0}^{\infty} \frac{1}{k!}\,(s^i\,W_i)^k = I_n + s^i\,W_i + \frac{1}{2}\,(s^i\,W_i)^2 + \frac{1}{3!}\,(s^i\,W_i)^3 + \ldots \quad ,$$

that is :

$$\exp(s^i\,W_i) = \begin{pmatrix} 0 & & & & & 0 \\ & \ddots & & & & \\ & & a^i_i & & & \\ & & & \ddots & & \\ 0 & & & & 0 & \end{pmatrix} \quad , \qquad (2.2.5)$$

where :

$$a^i_i = \sum_{k=0}^{\infty} \frac{1}{k!}\,(s^i\,\partial_i)^k \ . \qquad (2.2.6)$$

Applying $\exp(W_i)$ to a point of coordinates $u = (u^1;\,\ldots;\,u^n)$ in the n-dimensional Euclidean manifold, we obtain :

$$\exp(s^i\,W_i)\,u \ = \ I_n\,u + s^i\,W_i\,u + \underbrace{\frac{1}{2}\,(s^i\,W_i)^2\,u}_{=0} + \underbrace{\frac{1}{3!}\,(s^i\,W_i)^3\,u}_{=0} + \ldots \ = \ u + s^{(i)} \ , \quad (2.2.7)$$

where $s^{(i)} = (0;\,\ldots;\,s^i;\,\ldots;\,0)$, and notice that only the first two terms of the series contribute to the expression.

For a general vector $V \in \mathfrak{trans}(\mathbb{R}^n)$, where :

$$V = \sum_{i=1}^{n} s^i\,W_i \ \ ,$$

$s^1,\,\ldots,\,s^n$ being the components of V with respect to the canonical basis, we have :

$$\exp\left(\sum_{i=1}^{n} s^i\,W_i\right) = \prod_{i=1}^{n} \exp(s^i\,W_i) \ , \qquad (2.2.8)$$

as $[W_i\,;\,W_j] = 0_n$, for all $1 \leqslant i,j \leqslant n$. Then, as $\partial_i\partial_j u = 0$:

$$\exp\left(\sum_{i=1}^{n} s^i\,W_i\right)u \ = \ \prod_{i=1}^{n} \exp(s^i\,W_i)\,u \ = \ \prod_{i=1}^{n}(I_n + s^i\,W_i)\,u \ = \ \left(I_n + \sum_{i=1}^{n} s^i\,W_i\right)u \ .$$

In conclusion,

$$\exp\left(\sum_{i=1}^{n} s^i\,W_i\right)u = \bar{S}\,u \ , \qquad (2.2.9)$$

whereas $\exp\left(\sum_{i=1}^{n} s^i\,W_i\right)$ and the initial matrix $\bar{S}$ are not equal. We shall write

$$\bar{S} \equiv \exp\left(\sum_{i=1}^{n} s^i\,W_i\right)$$

and claim that they are equivalent, as their actions on the natural coordinates u of $\mathbb{R}^n$ yield the same result.

If we wish to avoid the notion of equivalence, we can simply define $\bar{S}$ as :

$$\bar{S} = \exp\left(\sum_{i=1}^{n} s^i W_i\right) \ ,$$

and conclude that the contribution of the first two terms of the series only is due to the fact that the considered manifold is Euclidean. This viewpoint is particularly interesting because it would possibly lead to the definition of a translation in a general manifold and not only in the Euclidean one. For that, we need to return to expression 2.1.12 and write it as :

$$u'^i = \sum_{j=1}^{n} \left(\delta^i_j + \delta^i_j \sum_{k=l}^{n} s^l \, \partial_l\right) u^j \ ; \tag{2.2.10}$$

In matrix notation :

$$u' = \left(I_n + I_n \sum_{l=1}^{n} s^l \, \partial_l\right) u \ . \tag{2.2.11}$$

A general Euclidean isometry is still represented by a matrix $\bar{F} = F + S$, where F is the usual matrix part; however, S has another form, it is the scalar matrix :

$$S = \begin{pmatrix} \sum_{l=1}^{n} s^l \, \partial_l & & 0 \\ & \ddots & \\ 0 & & \sum_{k=1}^{n} s^l \, \partial_l \end{pmatrix} \ . \tag{2.2.12}$$

In the case where $F = I_n$, the matrix $\bar{S} \doteq I_n + S$ corresponds to a pure translation. The set of all matrices $\bar{S}$ is then also noted $\mathrm{Trans}(\mathbb{R}^n)$, even if $\bar{S}$ has another shape than previously. Calculating the derivative of $\bar{S}$ with respect to s^i and taking its value at $s = 0$, we obtain :

$$\left.\frac{\partial \bar{S}}{\partial s^i}\right|_{s=0} \doteq W_i \ , \tag{2.2.13}$$

where :

$$W_i = \begin{pmatrix} \partial_i & & 0 \\ & \ddots & \\ 0 & & \partial_i \end{pmatrix} \ . \tag{2.2.14}$$

W_i is a tangent vector of $\mathrm{Trans}(\mathbb{R}^n)$ at the origin; the set $\{W_i \mid 1 \leqslant i \leqslant n\}$ constitutes the canonical basis of the tangent space of $\mathrm{Trans}(\mathbb{R}^n)$ at the origin. This space, also noted $\mathfrak{trans}(\mathbb{R}^n)$, has the structure of an algebra, as it is closed under the commutation operation :

$$[W_i; W_j] = 0_n \ , \quad \forall \ 1 \leqslant i, j \leqslant n \ . \tag{2.2.15}$$

Note that these commutation relations are the same as previously.

Let $V = \sum_{i=1}^{n} s^i W_i \in \mathfrak{trans}(\mathbb{R}^n)$, where $s^1, \ldots, s^n$ are the components of V in the canonical basis of $\mathfrak{trans}(\mathbb{R}^n)$; then :

$$\exp\left(\sum_{i=1}^{n} s^i W_i\right) = \sum_{k=0}^{\infty} \frac{1}{k!}\left(\sum_{i=1}^{n} s^i W_i\right)^k \ ,$$

hence :

$$\exp\left(\sum_{i=1}^{n} s^i\, W_i\right) = \begin{pmatrix} \exp\left(\sum_{i=1}^{n} s^i\, \partial_i\right) & & 0 \\ & \ddots & \\ 0 & & \exp\left(\sum_{i=1}^{n} s^i\, \partial_i\right) \end{pmatrix} \quad . \qquad (2.2.16)$$

This matrix is not equal to $\bar{S}$. However, the expressions resulting of its application to the natural coordinates u is equal to $\bar{S}\, u$, as :

$$\exp\left(\sum_{i=1}^{n} s^i\, \partial_i\right) u^i = \left[1 + \left(\sum_{i=1}^{n} s^i\, \partial_i\right) + \frac{1}{2}\left(\sum_{i=1}^{n} s^i\, \partial_i\right)^2 + \dots\right] u^i = u^i + s^i + 0 + \dots \quad ,$$

Thus, the matrix S can be replaced by $\tilde{S} \doteq I_n \exp\left(\sum_{i=1}^{n} s^i\, \partial_i\right)$ and $\mathrm{Trans}(\mathbb{R}^n)$ can be defined as :

$$\mathrm{Trans}(\mathbb{R}^n) = \left\{ \tilde{S} = I_n \exp\left(\sum_{i=1}^{n} s^i\, \partial_i\right) \;\middle|\; s^i \in \mathbb{R},\; 1 \leqslant i \leqslant n \right\} \quad . \qquad (2.2.17)$$

The interesting point is that $\mathrm{Trans}(\mathbb{R}^n)$ does not only generate translations in $\mathbb{R}^n$ but also in any manifold of dimension n embedded in $\mathbb{R}^m$, $m \geqslant n$. Indeed, let $M \subset \mathbb{R}^m$ be a manifold of dimension $n \leqslant m$, $\mathcal{U}$ an open set of M, $\tilde{\mathcal{U}}$ an open set of $\mathbb{R}^m$ and

$$\begin{aligned} H : \tilde{\mathcal{U}} &\longrightarrow \quad \mathcal{U} \subset M \\ u &\longmapsto \quad H(u) \;, \end{aligned}$$

$u = (u^1;\, \dots;\, u^n)$ and $H = (h^1;\, \dots;\, h^m)$, a local parameterisation of M. Then :

$$\exp\left(\sum_{l=1}^{n} s^l\, \partial_l\right) h^i(u) = h^i(u) + \sum_{l=1}^{n} s^l\, \frac{\partial h^i(u)}{\partial u^l} + \frac{1}{2} \sum_{l_1,\, l_2 = 1}^{n} s^{l_1}\, s^{l_2}\, \frac{\partial^2 h^i(u)}{\partial u^{l_1}\, \partial u^{l_2}} + \dots$$

$$+ \frac{1}{r!} \sum_{l_1,\, \dots,\, l_r = 1}^{n} s^{l_1} \dots s^{l_r}\, \frac{\partial^r h^i(u)}{\partial u^{l_1} \dots \partial u^{l_r}} + \dots$$

This expression is exactly the Taylor expansion of h^i in a neighbourhood of a point with natural coordinates u, provided $H(u+s) \in \mathcal{U}$. Thus :

$$\exp\left(\sum_{l=1}^{n} s^l\, \partial_l\right) h^i(u) = h^i(u+s) \;, \qquad (2.2.18)$$

the matrix $\tilde{S}$ carries the point $H(u)$ of M to the point $H(u+s)$ which also belongs to M. Note that $\tilde{S}$ is still an $m \times m$ and not $n \times n$ matrix, even if the dimension of the manifold is $m \leqslant n$.

All these important results are summarised and illustrated in the following definition, lemma, consequence and example.

2.2.1 Definition : Let $\mathbb{R}^n$ be the n-dimensional Euclidean manifold endowed with the natural coordinate system $u = (u^1; \ldots; u^n)$. The set

$$\text{Trans}(\mathbb{R}^n) = \left\{ \tilde{S} = I_n \exp\left(\sum_{l=1}^{n} s^l \, \partial_l \right) \, \bigg| \, s^l \in \mathbb{R} \text{ and } \partial_l = \frac{\partial}{\partial u^l} \, , \, 1 \leqslant l \leqslant n \right\}$$

is called the *translation group of* $\mathbb{R}^n$ (or the *group of matrix operators representing the translations in* $\mathbb{R}^n$). Any element acts on points of $\mathbb{R}^n$, with coordinates u, as :

$$u \; \longmapsto \; \tilde{S} \, u = u + s \; ,$$

where $s = (s^1; \ldots; s^n)$.

2.2.2 Lemma : $\text{Trans}(\mathbb{R}^n)$ *is a Lie group, i.e. a smooth manifold that is also a group, parameterised by the map* :

$$(s^1; \ldots; s^n) \; \longmapsto \; I_n \exp\left(\sum_{l=1}^{n} s^l \, \partial_l \right) \; . \tag{2.2.19}$$

The set

$$\mathfrak{trans}(\mathbb{R}^n) = \left\{ V = \sum_{i=1}^{n} s^i \, W_i \, \bigg| \, W_i = I_n \, \partial_i \, , \; 1 \leqslant i \leqslant n \right\}$$

has the structure of an algebra and is called Lie algebra associated with the Lie group $\text{Trans}(\mathbb{R}^n)$. *The matrices* W_i *can be obtained from* $\tilde{S}$ *by calculating the derivative of* $\tilde{S}$ *with respect to* s^i *and taking its at* $s = 0$:

$$W_i = \left. \frac{\partial \tilde{S}}{\partial s^i} \right|_{s=0} \; .$$

$\mathfrak{trans}(\mathbb{R}^n)$ *is nothing else than the tangent space of* $\text{Trans}(\mathbb{R}^n)$ *at the origin. The set of matrices* $\{ W_i \mid l \leqslant i \leqslant n \}$ *form a basis of this space; it is the canonical basis associated with the parameterisation 2.2.19.*

2.2.3 Consequence : Let M be a manifold of dimension n embedded in $\mathbb{R}^m$, $n \leqslant m$. Let $\mathcal{U} \subset M, \tilde{\mathcal{U}} \subset \mathbb{R}^n$ be two open sets, and

$$\begin{aligned} H : \tilde{\mathcal{U}} &\longrightarrow \quad \mathcal{U} \\ u &\longmapsto \quad H(u) \; , \end{aligned}$$

$u = (u^1; \ldots; u^n)$ and $H = (h^1; \ldots; h^m)$, a local parameterisation of M. Then, any element of the set

$$\text{Trans}(M) = \left\{ \tilde{S} = I_m \exp\left(\sum_{l=1}^{n} s^l \, \partial_l \right) \, \bigg| \, s^l \in \mathbb{R} \text{ and } \partial_l = \frac{\partial}{\partial u^l} \, , \, 1 \leqslant l \leqslant n \right\}$$

generates a translation in M provided $H(u + s) \in \mathcal{U}$ when $H(u) \in \mathcal{U}$. $\text{Trans}(M)$ and $\text{Trans}(\mathbb{R}^n)$ are almost the same, the only difference is in the size of the identity matrix.

2.2.4 Remark : Trans(M) has not truly the structure of a group, since certain elements of Trans(M) carry points of $\mathcal{U} \subset M$ outside $\mathcal{U}$, which is not defined. This problem does not concern us, as we shall henceforth only consider manifolds which can be parameterised by one one-to-one map $H : \mathbb{R}^n \to M$. In such a case, Trans(M) is a group and is called *translation group of* M (or *groupe of translations of* M).

2.2.5 Example : Let $\mathbb{S}^2 \subset \mathbb{R}^3$ be the two-dimensional sphere of radius R, parameterised by the map :

$$(\theta; \varphi) \longmapsto (R\sin\theta\cos\varphi; \ R\sin\theta\sin\varphi; \ R\cos\theta) \ .$$

Any element of its translation group can be written as :

$$\tilde{S} = I_3 \exp(s^\theta \, \partial_\theta + s^\varphi \, \partial_\varphi) \ ,$$

where $\partial_\theta = \frac{\partial}{\partial\theta}$ and $\partial_\varphi = \frac{\partial}{\partial\varphi}$. In the particular case where $s^\varphi = 0$, we have :

$$\tilde{S} = I_3 \exp(s^\theta \, \partial_\theta) = I_3 \sum_{k=0}^{\infty} \frac{(s^\theta \, \partial_\theta)^k}{k!} \quad .$$

Applying this matrix to points of $\mathbb{S}^2$, for example the north pole $(0; 0; R)$, we obtain :

$$\begin{pmatrix} \exp(s^\theta \, \partial_\theta) & 0 & 0 \\ 0 & \exp(s^\theta \, \partial_\theta) & 0 \\ 0 & 0 & \exp(s^\theta \, \partial_\theta) \end{pmatrix} \begin{pmatrix} R\sin\theta\cos\varphi \\ R\sin\theta\sin\varphi \\ R\cos\theta \end{pmatrix}_{(\theta;\varphi)=(0;0)} =$$

$$= \begin{pmatrix} 0 \\ 0 \\ R \end{pmatrix} + s^\theta \begin{pmatrix} R \\ 0 \\ 0 \end{pmatrix} + \frac{(s^\theta)^2}{2!} \begin{pmatrix} 0 \\ 0 \\ -R \end{pmatrix} + \frac{(s^\theta)^3}{3!} \begin{pmatrix} -R \\ 0 \\ 0 \end{pmatrix} + \frac{(s^\theta)^4}{4!} \begin{pmatrix} 0 \\ 0 \\ R \end{pmatrix} + \dots =$$

We recognise terms of the sinus series in the first component and terms of the cosinus series in the third one. Thus :

$$\begin{pmatrix} \exp(s^\theta \, \partial_\theta) & 0 & 0 \\ 0 & \exp(s^\theta \, \partial_\theta) & 0 \\ 0 & 0 & \exp(s^\theta \, \partial_\theta) \end{pmatrix} \begin{pmatrix} R\sin\theta\cos\varphi \\ R\sin\theta\sin\varphi \\ R\cos\theta \end{pmatrix}_{(0;0)} = \begin{pmatrix} R\sin s^\theta \\ 0 \\ R\cos s^\theta \end{pmatrix} \quad .$$

This last expression corresponds to the coordinates of a point on the sphere which lies on a meridian. Its distance from the north pole is equal to the length of the curve on this meridian linking these points :

$$\ell = \int_0^{s^\theta} R \, \mathrm{d}t = R \, s^\theta \quad .$$

Note that when s^θ is bigger than $2\,\pi$, the curve which
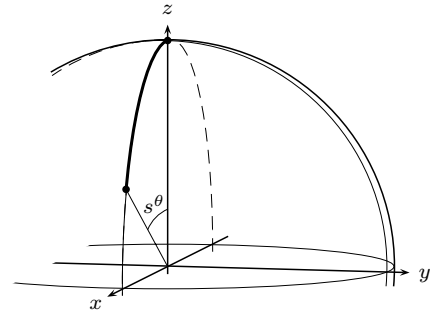
starts at the north pole and follows the meridian goes again through the north pole before reaching the endpoint. This situation in fact never happens if we require the appropriate restrictions on θ and φ, that is $\theta \in [0\,;\,\pi]$ and $\varphi \in [0\,;\,2\pi[$, in order to have a real parameterisation, that is a diffeomorphism between $[0\,;\,\pi] \times [0\,;\,2\pi[$ and $\mathbb{S}^2$.

2.2.2 Action of a One-parameter Translation Group on a Manifold

The action of a group on a vector space is a concept relatively well known, as it is directly connected to *representation theory*. However, it must be borne in mind that the notion of action of a group is not limited to vector spaces; important applications also exist in the case of manifolds.

2.2.6 Definition : Let $(\mathcal{G}\,;\,\diamond)$ be a group, with internal composition operation $\diamond$ and neutral element e, and M a manifold. A *(left) action of $\mathcal{G}$ on M* is a map :

$$\begin{aligned} \mu :\ \mathcal{G} \times M\ &\longrightarrow\ M \\ (g;\,p)\ &\longmapsto\ \mu(g;\,p) \end{aligned}$$

which satisfies the following conditions

$$\mu(e;\,p) = p\,, \qquad\qquad \forall\,p \in M\,,$$

$$\mu\big(g_2;\,\mu(g_1;\,p)\big) = \mu\big((g_2 \diamond g_1)\,;\,p\big)\,, \quad \forall\,p \in M, \quad \forall\,g_1,\,g_2 \in \mathcal{G}\,.$$

For the translation group, its action on a manifold M is defined as follows :

2.2.7 Definition : Let $M \subset \mathbb{R}^m$ be an n-dimensional smooth manifold parameterised by the smooth map $H : \mathbb{R}^n \to M$, $H = (h^1;\,\ldots;\,h^m)$. The (left) action μ_{T} of the group of translation $\mathrm{Trans}(M)$ (see definition 2.2.1) on M is given by :

$$\begin{aligned} \mu_{\mathrm{T}} :\ \mathrm{Trans}(M) \times M\ &\longrightarrow\ M \\ \big(\tilde{S};\,H(u)\big)\ &\longmapsto\ \mu_{\mathrm{T}}\big(\tilde{S};\,H(u)\big) = \tilde{S}\,H(u)\,, \end{aligned}$$

where $H(u)$ is the column-vector composed of $h^1(u)$, $\ldots$, $h^m(u)$. Note that $H(u)$ corresponds to the natural coordinates in $\mathbb{R}^m$ of a point in M.

Note that this definition has in fact already been indirectly mentioned previously, in consequence 2.2.3.

2.2.8 Remark : Using the Taylor series, we have :

$$\tilde{S}\,H(u) = H(u + s)\,.$$

We can then write :

$$\tilde{S}\,H(u) = \big(H \circ T \circ H^{-1}\big)\big(H(u)\big)\,,$$

where T is given by $T(u) = \tilde{S}\,u$. The action of $\mathrm{Trans}(M)$ on M could therefore be defined as :

$$\big(\tilde{S};\, H(u)\big) \longmapsto \big(H \circ T \circ H^{-1}\big)\big(H(u)\big) = H(\tilde{S}\,u)\ .$$

Rigorously speaking, $\mathrm{Trans}(M)$ is not directly the translation group of the manifold M, but its matrix representation. Elements of this group can also be represented by $H \circ T \circ H^{-1}$, the action of which is defined just above.

In Lie theory, important subgroups of Lie groups are the so-called *one-parameter subgroups.* According to definitions B.3.1, B.3.2, B.3.4 and lemma B.3.3 (see appendix B), a one-parameter subgroup in a Lie group $\mathcal{G}$ is a smooth curve γ such that $\gamma(t_1 + t_2) = \gamma(t_1)\,\gamma(t_2)$, which corresponds to a maximal integral curve of the elements of the associated Lie algebra $\mathfrak{g}$, which start at the neutral element e of the group. The *Lie exponential map* carries elements V of the Lie algebra $\mathfrak{g}$ to $\gamma_V(1) \in \mathcal{G}$ and $t \mapsto \exp(t\,V)$ is the one-parameter subgroup generated by V. In the case where the considered Lie group is $\mathrm{GL}_n(\mathbb{R})$, the set of all $n \times n$ invertible matrices, the Lie exponential map is the map $\exp$ given by its power series $\exp V = \sum_{k=0}^{\infty} \frac{V^k}{k!}$. A formal extension of these results to the translation group leads to the following considerations :

2.2.9 Definition : The one-parameter subgroups in $\mathrm{Trans}(M)$ are :

$$
\begin{aligned}
\mathbb{R} &\longrightarrow \mathrm{Trans}(M)\\
t &\longmapsto \exp(t\,V)\ ,
\end{aligned}
$$

where :

$$V = \sum_{j=1}^{n} s^j\,W_j\ , \quad \text{with } W_j = I_m\,\partial_j\ .$$

When $t = 1$, we have $\exp(V)$, that is $\tilde{S}$, the matrix associated with the translation s.

2.2.10 Definition : The (left) action of a one-parameter subgroup of $\mathrm{Trans}(M)$ on a point of the manifold M, the coordinates of which are $H(u)$ is :

$$\big(\exp(t\,V);\, H(u)\big) \longmapsto \exp(t\,V)\,H(u) = H(u + s\,t)\ ,$$

where $s = (s^1;\, \dots;\, s^n)$. Thus, a one-parameter subgroup of translations, that is a curve in $\mathrm{Trans}(M)$, generates a curve in M.

2.2.3   Infinitesimal Translation and Tangent Space

Let $t \mapsto \exp(t\,V)\,H(u) \subset M$ a curve going through the point $H(u)$, generated by the one-parameter subgroup $t \mapsto \exp(t\,V) \subset \mathrm{Trans}(M)$, $V = \sum_{j=1}^{n} s^j\,W_j = I_m \sum_{j=1}^{n} s^j\,\partial_j$, on $H(u)$. A point of the curve infinitely close to $H(u)$ is given by

$$\exp(\mathrm{d}t\,V)\,H(u) = H(u + s\,\mathrm{d}t)\ , \tag{2.2.20}$$

where $\mathrm{d}t$ is an infinitesimal element of t. Using the Taylor development, we obtain :

$$H(u + s\,\mathrm{d}t) \cong H(u) + \sum_{j=1}^{n} \frac{\partial H}{\partial u^j}(u)\, s^j\, \mathrm{d}t \qquad (2.2.21\mathrm{a})$$

in components :

$$h^i(u + s\,\mathrm{d}t) \cong h^i(u) + \sum_{j=1}^{n} \frac{\partial h^i}{\partial u^j}(u)\, s^j\, \mathrm{d}t \ . \qquad (2.2.21\mathrm{b})$$

As $\mathrm{d}t$ is very small, the terms of higher order are negligible. These two last expressions can also be obtained by considering the exponential map series and keeping only the zero and first order terms (the other being negligible) :

$$\exp(\mathrm{d}t\, V) \cong I_m + \mathrm{d}t\, V \ . \qquad (2.2.22)$$

The point of coordinates $H(u + s\,\mathrm{d}t)$ can be seen as the tip of a tangent vector at the point of coordinates $H(u)$. Indeed, the tangent vector of the curve $t \mapsto H(u + s\,t)$ at the point of coordinates $H(u)$ is :

$$v = \frac{\mathrm{d}}{\mathrm{d}t} H(u + s\,t)\big|_{t=0} = \sum_{j=1}^{n} \frac{\partial H}{\partial u^j}(u)\, s^j \ ; \qquad (2.2.23\mathrm{a})$$

in components :

$$v^i = \frac{\mathrm{d}}{\mathrm{d}t} h^i(u + s\,t)\big|_{t=0} = \sum_{j=1}^{n} \frac{\partial h^i}{\partial u^j}(u)\, s^j \ . \qquad (2.2.23\mathrm{b})$$

Multiplying these relations by $\mathrm{d}t$, we obtain an infinitesimal tangent vector at the point of coordinates $H(u)$, with the same direction as v :

$$v\,\mathrm{d}t = \sum_{j=1}^{n} \frac{\partial H(u)}{\partial u^j}(u)\, s^j\, \mathrm{d}t \ ; \qquad (2.2.24\mathrm{a})$$

in components :

$$v^i\,\mathrm{d}t = \sum_{j=1}^{n} \frac{\partial h^i(u)}{\partial u^j}(u)\, s^j\, \mathrm{d}t \ ; \qquad (2.2.24\mathrm{b})$$

$v\,\mathrm{d}t$ is exactly the second term of the Taylor development 2.2.21a.

Expression 2.2.23a), which can be written as :

$$v = \sum_{j=1}^{n} s^j\, \partial_j\, H(u) = \sum_{j=1}^{n} s^j\, W_j\, H(u) \ , \qquad (2.2.25)$$

where $W_j = I_m \, \partial_j$, shows that a vector of the Lie algebra $\mathfrak{trans}(M)$ generates a vector in the tangent space of M at the point of coordinates $H(u)$. In particular, any basis vector $W_i \in \mathfrak{trans}(M)$ generates the vector :

$$w_i = W_i \, H(u) = \frac{\partial H}{\partial u^i}(u) \,, \tag{2.2.26}$$

which is the i-th canonical basis vector of the tangent space of M at the point of coordinates $H(u)$, associated with the parameterisation H. As any tangent space to M has the same dimension as the Lie algebra $\mathfrak{trans}(M)$, we conclude that the map which assigns any canonical basis vector $W_i \in \mathfrak{trans}(M)$ to the canonical basis vector w_i of the tangent space of M at the point of coordinates $H(u)$ is linear and one-to-one. Thus :

2.2.11 Lemma : *The Lie algebra $\mathfrak{trans}(M)$, seen as a vector space, and any tangent space of M are isomorphic.*

2.2.4   Lattice in a Manifold and in its Tangent Spaces

The derivations done in the previous subsection show that an infinitesimal translation, belonging to the Lie algebra $\mathfrak{trans}(M)$, generates in the manifold M a point very close to the initial point, which can be seen as the tip of a tangent vector of M at the initial point. When the translation is not infinitesimal, this result does not hold any more in general. Indeed, consider the (smooth) curve :

$$\begin{aligned} [0\,;1] &\longrightarrow \mathfrak{trans}(M) \\ t &\longmapsto t\,V = t\sum_{j=1}^{n} s^j \, W_j \,. \end{aligned}$$

The Lie exponential map carries this curve to a curve in the translation group

$$\begin{aligned} [0\,;1] &\longrightarrow \mathrm{Trans}(M) \\ t &\longmapsto \exp(t\,V) = \exp\!\left(t\sum_{j=1}^{n} s^j \, W_j\right) \end{aligned}$$

which generates a curve in the manifold M :

$$\begin{aligned} [0\,;1] &\longrightarrow M \\ t &\longmapsto \exp(t\,V)\,H(u) = H(u + s\,t) \,. \end{aligned}$$

The tangent vector to this curve at the starting point, with coordinates $H(u)$, is :

$$v = \sum_{j=1}^{n} \frac{\partial H}{\partial u^j}(u)\, s^j \,, \tag{2.2.27}$$

and is not equal to $H(u + s)$ in general. However, even if it is not equal, a one-to-one correspondence between $H(u + s)$ and v can be exhibited. Indeed, since the derivative

of a (smooth) map at a point is unique, the tangent vector of a curve at a point is also unique. Reciprocally, let $t \mapsto H(u + r\,t)$, $r \in \mathbb{R}^n$ be a family of curves which intersect only at $H(u)$; for a given vector v in the tangent space at the point of coordinates $H(u)$, there is, among these curves, exactly one, the tangent vector of which at $t = 0$ is v. This vector v can also be obtained when applying the vector $V \in \mathfrak{trans}(M)$ (that is the endpoint of the curve $t \mapsto t\,V$ parameterised between 0 and 1) to $H(u)$:

$$V\,H(u) = \sum_{j=1}^{n} s^j\,W_j\,H(u) = \sum_{j=1}^{n} s^j\,\frac{\partial H}{\partial u^j}(u) = v \ . \tag{2.2.28}$$

All these considerations can be summarised as follows.

2.2.12 Theorem : *Let $\mathbb{R}^n$ and $\mathbb{R}^m$, $m \geqslant n$, be respectively the n and m-dimensional Euclidean spaces, and $M \subset \mathbb{R}^m$ a smooth manifold of dimension n, parameterised by the diffeomorphism $H : \mathbb{R}^n \to M$, $H = (h^1; \ldots; h^m)$. Let $\mathrm{T}_p M$ be the tangent space of M at the point p of coordinates $H(u_p)$. Let $\mathrm{Trans}(M)$ be the translation group of M and $\mathfrak{trans}(M)$ its Lie algebra. Then :*

$$
\begin{array}{ccc}
 & \mathbb{R}^n & \\
 & \Big| \cong & \\
 & \downarrow & \\
 & \mathfrak{trans}(M) & \\
{}^{\exp}\swarrow & & \searrow^{\cong} \\
\mathrm{Trans}(M) & & \mathrm{T}_p M \\
{}_{act_{H(u_p)}}\searrow & & \swarrow_{\widetilde{\exp}} \\
 & M &
\end{array}
$$

where :
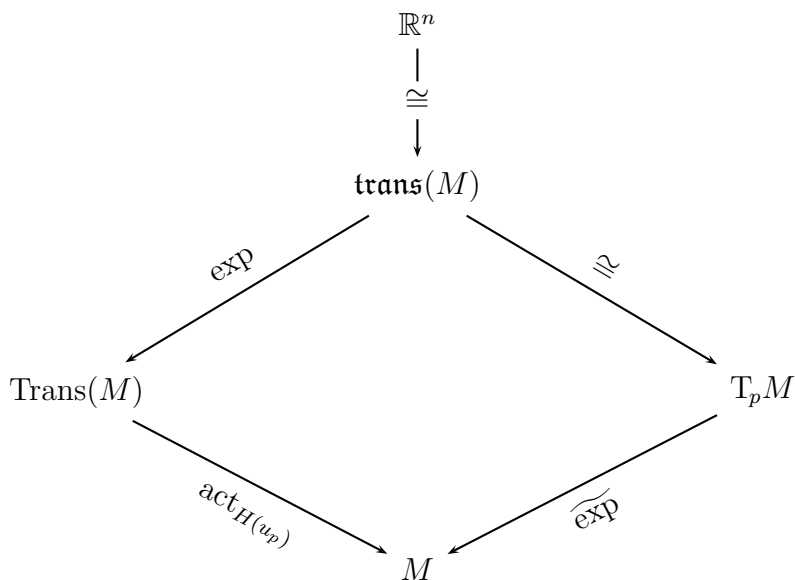
$$
\begin{aligned}
\exp : \mathfrak{trans}(M) &\longrightarrow \mathrm{Trans}(M) \\
V &\longmapsto \tilde{S} = \exp(V) \ , \qquad V = \sum_{j=1}^{n} s^j\,W_j \ ,
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{act}_{H(u_p)} : \mathrm{Trans}(M) &\longrightarrow M \\
\tilde{S} &\longmapsto \tilde{S}\,H(u_p) \ ,
\end{aligned}
$$

and

$$\widetilde{\exp} : \qquad \mathrm{T}_p M \qquad \longrightarrow \qquad M$$
$$\left(I_m \sum_{j=1}^{n} s^j\, \partial_j \right) H(u) \big|_p \;\; \longmapsto \;\; \exp\left(I_m \sum_{j=1}^{n} s^j\, \partial_j \right) H(u) \big|_p \;.$$

$\mathfrak{trans}(M)$ and $\mathrm{T}_p M$ are isomorphic through the map :

$$\sum_{j=1}^{n} s^j\, W_j \;\; \longmapsto \;\; \sum_{j=1}^{n} s^j\, W_j\, H(u) \big|_p \;,$$

as well as $\mathbb{R}^n$, seen as a vector space, and $\mathfrak{trans}(M)$, through the map :

$$(s^1;\, \ldots;\, s^n) \;\; \longmapsto \;\; \sum_{j=1}^{n} s^j\, W_j \;.$$

It is important to keep in mind the notion of one-parameter subgroup in $\mathrm{Trans}(M)$ and curve in M, even if it does not concretely appear in the previous theorem. The $\widetilde{\exp}$ map carries any vector $v \in \mathrm{T}_p M$ into the point $\gamma_v(1)$ of the curve $t \mapsto \gamma_v(t)$, the expression in coordinates of which is $t \mapsto H(u_p + s\,t)$, and the tangent vector of which is v at $H(u_p)$. As mentioned earlier, there is a one-to-one correspondance between tangent vectors at a point of coordinates $H(u)$ and curves belonging to the family of curves, the expression in coordinates of which is $t \mapsto H(u + r\,t)$, where $r \in \mathbb{R}^n$. This is due to the fact that there is exactly one straight line linking two points in $\mathbb{R}^n$, and that H is one-to-one. But this does not mean that there is a one-to-one correspondance between tangent vectors v and points $\gamma_v(1)$. This is typically not the case when M is a compact manifold. For instance, on the sphere $\mathbb{S}^2$, an infinity of curves (belonging to the same family, the meridians in this case) link the north to the south poles. Thus, to one point, the south pole, corresponds an infinity of tangent vectors in the tangent space at the north pole, whereas there is only one tangent vector at the north pole which is the tangent vector of a given meridian (linking the north to the south poles).

The previous theorem has an interesting application when a finite free $\mathbb{Z}$-module in $\mathbb{R}^n$ is considered.

2.2.13 Corollary : Let $M \subset \mathbb{R}^m$ be a manifold parameterised by a diffeomorphism $H : \mathbb{R}^n \to M$, $H = (h^1;\, \ldots;\, h^m)$, and $\mathrm{T}_p M$ its tangent space at the point p of coordinates $H(u_p)$. Let $\mathrm{Trans}(M)$ be the group of translations of M and $\mathfrak{trans}(M)$ its Lie algebra. Let

$$\mathbb{Z}^n_B = \{ B\,\lambda \mid \lambda \in \mathbb{Z}^n \}$$

where $B \in \mathrm{GL}_n(\mathbb{R})$ be an n-dimensional finite free $\mathbb{Z}$-module in $\mathbb{R}^n$. To this module corresponds an n-dimensional finite free $\mathbb{Z}$-module in $\mathfrak{trans}(M)$

$$\mathfrak{Z}^n_B = \left\{ \sum_{j=1}^{n} (B\,\lambda)^j\, W_j \;\middle|\; \lambda \in \mathbb{Z}^n \right\} \;,$$

which generates an n-dimensional finite free $\mathbb{Z}$-module

$$\Upsilon_p = \left\{ \sum_{j=1}^{n} \frac{\partial H}{\partial u^j}(u_p)\,(B\,\lambda)^j \,\middle|\, \lambda \in \mathbb{Z}^n \right\}$$

in T_pM and a discrete subset

$$\tilde{\Lambda} = \{ H(u_p + B\,\lambda) \mid \lambda \in \mathbb{Z}^n \}$$

in M. These results can be summarised in the following diagram :

$$
\begin{array}{ccc}
 & \mathbb{Z}_B^n & \\
 & \Big| \cong & \\
 & \mathfrak{Z}_B^n & \\
\text{exp} \swarrow & & \searrow \cong \\
\exp(\mathfrak{Z}_B^n) & & \Upsilon_p \\
act_{H(u_p)} \searrow & & \swarrow \widetilde{\exp} \\
 & \tilde{\Lambda} &
\end{array}
$$
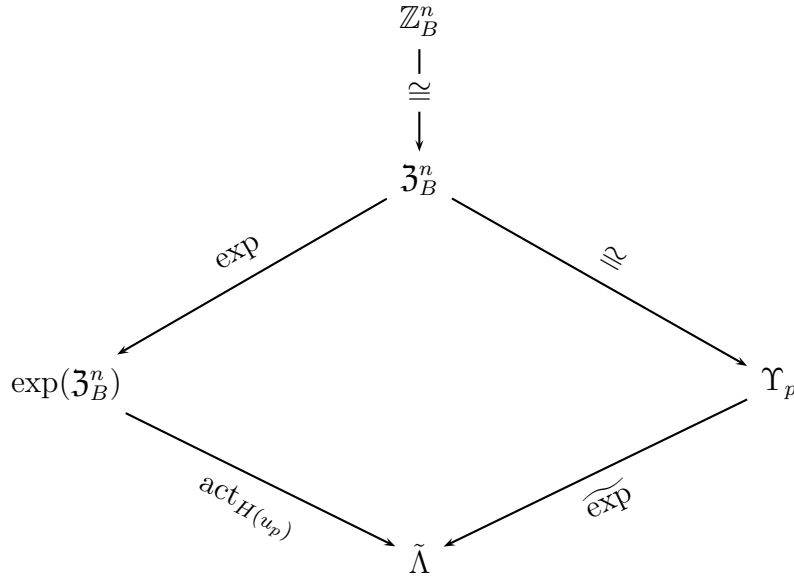
2.2.14 Definition : The discrete subset $\tilde{\Lambda}$ will be called *lattice in the manifold M* and the finite free $\mathbb{Z}$-module Υ_p its *representation in the tangent space T_pM*.

2.2.15 Remark : Note that the same lattice $\tilde{\Lambda} \subset M$ can be obtained when starting with the $\mathbb{Z}$-module $\mathbb{Z}^n \subset \mathbb{R}^n$. Indeed, if we consider a parameterisation $\tilde{H} = H \circ B$, we effectively find

$$\exp\left(\sum_{j=1}^{n} \lambda^j\, W_j' \right) \tilde{H}(x_p) = \tilde{H}(x_p + \lambda) = H(B\,x_p + B\,\lambda) = H(u_p + B\,\lambda) \ .$$

where $u = B\,x$ and W' is referred to the variables $x = (x^1; \ldots; x^n)$. Thus, one can equivalently start with a *square lattice* $\mathbb{Z}^n \subset \mathbb{R}^n$ which then generates a lattice $\mathbb{Z}^n$ distorted by the map $\tilde{H} = H \circ B$, or directly consider the more general module $\mathbb{Z}_B^n$ which generates a lattice $B\,\mathbb{Z}^n$ distorted by the map H. The important point is to obtain the same geometrical features in M and T_pM. In $\mathfrak{trans}(M)$, as no scalar product is defined, no concrete geometry is considered, hence the choice of the module in this space is not important.

2.3   Point space and associated vector space*s*

The theory and results presented up to this point are a pre-requirement for the treatment of crystal structures including modulated ones. The main point that should be kept in mind is that the group of translations does not generate vectors or straight lines only, but also and especially curves. In fact, the group of translations generates vectors in any tangent space of a manifold M but never in M directly. It is important to realise that manifolds are not vector spaces. Even the Euclidean space, the properties of which are very close to those of vector spaces, is a manifold and not a vector space; any map of its isometry group is not linear but affine. Any two points on a connected manifold can be linked by a curve, but usually not by a vector. For instance, the trajectory of a boat sailing from Port Ellen (Scotland) to Port Fairy (Australia) is not a straight line (it is not digging a tunnel through Earth) but a curve on the surface of our planet (this curve is usually of minimal length when there is no continent or isle between the starting and end points, in absence of storm, and (last, but not least) unless the captain has indulged too much in Caol Ila).

2.3.1   Structures in the Euclidean Manifold

In manifold theory, vectors are elements of tangent spaces, which are vector spaces, not of manifolds. The question is why vectors and not curves are always used for linking two points in the Euclidean manifold. To answer this question, we need the notions of *geodesic* and *exponential map*. A precise definition of a geodesic would require the introduction of concepts such as the *Levi-Civita connection*, the *covariant derivative* and the *parallel translation*. These concepts are presented in any textbook treating differential geometry, for instance in B. O'Neill's monograph [O'N83]; they will not be repeated here because they will not be used further.

Briefly, a geodesic on a Riemannian manifold is a curve which can be defined from one of its more important properties, namely that of being a curve of minimal length; for any two points in a connected Riemannian manifold without boundary, the curve of minimal length linking these two points is a geodesic. For example, geodesics are straight lines in the Euclidean space and arcs of great circles on the sphere $\mathbb{S}^2$ (for more details, see reference [O'N83]).

Let γ_v be the maximal geodesic (*i.e.* it cannot be extended) on a Riemannian manifold M such that $\gamma_v(0) = p \in M$, $\frac{\mathrm{d}\gamma_v}{\mathrm{d}t}(0) = \dot{\gamma}_v(0) = v$,
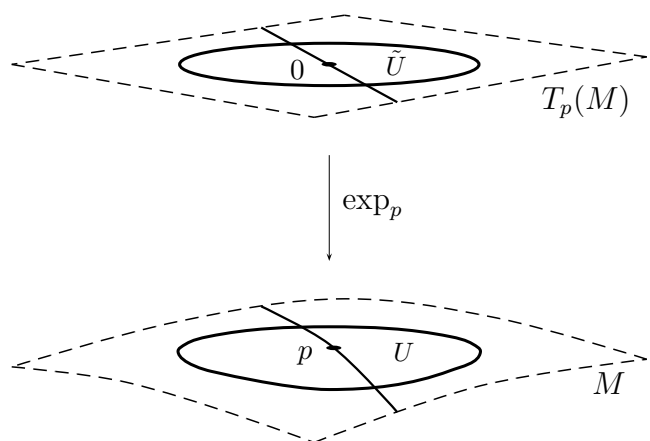

Figure 2.1: Illustration of the exponential map. It carries lines through the origin of $\mathrm{T}_p M$ to geodesics of M through p.

and $\widetilde{\mathrm{T}_p M}$ the set of all vectors v of $\mathrm{T}_p M$ such that γ_v is defined at least on $[0\,;1]$. Then, the *exponential map* of M at p is the function

$$
\begin{aligned}
\exp_p : \widetilde{\mathrm{T}_p M} &\longrightarrow M \\
v &\longmapsto \exp_p(v) = \gamma_v(1) \ .
\end{aligned}
$$

For a fixed v, $\exp_p(t\,v) = \gamma_{tv}(1) = \gamma_v(t)$, where $t \in \mathbb{R}$. Thus the exponential map $\exp_p$ carries lines through the origin of $\mathrm{T}_p M$ to geodesics of M through p (see figure 2.1). Note that for each point $p \in M$, there exists a neighbourhood $\tilde{\mathcal{U}}$ of 0 in $\mathrm{T}_p M$ on which the exponential map $\exp_p$ is a diffeomorphism onto a neighbourhood $\mathcal{U}$ of p in M. In several simple cases, for instance in the Euclidean space, $\tilde{\mathcal{U}} = \mathrm{T}_p M$ and $\mathcal{U} = M$. Note that the name of the exponential map comes from the theory of Lie groups; in the same way as exp carries lines through the origin of the Lie algebra to one-parameter subgroups of the Lie group, so does its geometrical analogue between lines through the origin of $\mathrm{T}_p M$ and geodesics through p in M.

Let us consider the n-dimensional Euclidean space $\mathbb{R}^n$ endowed with its natural coordinate system $u = (u^1;\,\ldots;\,u^n)$, in which the components of the metric tensor are $g_{ij}(p) = \delta_{ij}$, for all $p \in \mathbb{R}^n$, $1 \leqslant i,j \leqslant n$. The parameterisation H corresponds then to the identity map in this case. As written above, geodesics in this space are straight lines. Take two points q and p in $\mathbb{R}^n$ with coordinates $u_q = (u_q{}^1;\,\ldots;\,u_q{}^n)$ and $u_p = (u_p{}^1;\,\ldots;\,u_p{}^n)$ respectively. They are linked by a unique geodesic, a straight line. This geodesic, *linearly* parameterised between 0 and 1 (*i.e.* with a constant "velocity") is given by :

$$
\begin{aligned}
\gamma : \quad [0\,;1] &\longrightarrow \mathbb{R}^n \\
t &\longmapsto \gamma(t) = u_q + (u_p - u_q)\,t \ ,
\end{aligned}
$$

with $\gamma(0) = u_q$ and $\gamma(1) = u_p$; its tangent vector at q is :

$$
\frac{\mathrm{d}\gamma(t)}{\mathrm{d}t}\bigg|_{t=0} = \dot{\gamma}(0) = u_p - u_q \doteq v \ , \tag{2.3.1a}
$$

in components :

$$
v^i = u_p{}^i - u_q{}^i \ , \qquad 1 \leqslant i \leqslant n \ . \tag{2.3.1b}
$$

This vector and the starting point $\gamma(0) = u_q$ completely characterise the curve γ, which will then be noted γ_v; indeed, one can write :

$$
\gamma_v(t) = u_q + v\,t \ . \tag{2.3.2}
$$

γ_v is in fact generated by a (closed) subset of the one-parameter subgroup (*i.e.* a curve) of the translation group :

$$
\begin{aligned}
[0\,;1] &\longrightarrow \mathrm{Trans}(\mathbb{R}^n) \\
t &\longmapsto I_n \exp\left(t \sum_{j=1}^{n} v^j\,\partial_j \right) \quad ;
\end{aligned}
$$

the endpoint of this latter generates the endpoint p of γ_v. Note that as $\partial_i \partial_j u = 0$, for all $1 \leqslant i, j \leqslant n$, only the two first terms of the exponential series bring a non-zero contribution. Notice also that the components of the vector in $\mathfrak{trans}(M)$ generating this subgroup are the same as those of the tangent vector to γ_v at q. Expression 2.3.2 shows that the endpoint of γ_v, namely p, with coordinates $\gamma_v(1) = u_p$, can be seen as the tip of the tangent vector of the curve γ at q :

$$u_p = \gamma_v(1) = \underbrace{u_q}_{\in \mathbb{R}^n} + \underbrace{v}_{\in \mathrm{T}_q\mathbb{R}^n} \ . \tag{2.3.3}$$

In the case where q is the origin point o of the coordinate system (with coordinates $u_o = (0; \ldots; 0) = 0$), we have $u_p = \gamma_v(1) = u_o + v = v$, which can be written as $\exp_o(v) = v$. Even if this expression is perfectly correct, one should not forget that $\gamma_v(1)$ is a point of $\mathbb{R}^n$ whereas v is an element of $\mathrm{T}_o\mathbb{R}^n$. This result is fundamental because it shows that $\mathrm{T}_o\mathbb{R}^n$ and $\mathbb{R}^n$ are not only isomorphic but also *geometrically equivalent*, that is *isometric*, the isomorphism being the exponential map. [Also note that the metric tensor, the components of which in the natural coordinate system are δ_{ij}, $1 \leqslant i, j \leqslant n$, is constant and equal to the scalar product it generates in the tangent space.]

As an example, let us consider an n-dimensional (periodic) lattice Λ in the Euclidean space $\mathbb{R}^n$. To construct it, we consider the finite free $\mathbb{Z}$-module

$$\mathfrak{Z}_B^n = \left\{ \sum_{j=1}^{n} (B\,\lambda)^j\, W_j \,\middle|\, \lambda \in \mathbb{Z}^n \right\} , \quad \text{with } B \in \mathrm{GL}_n(\mathbb{R}) \text{ fixed}, \tag{2.3.4}$$

in the Lie algebra $\mathfrak{trans}(\mathbb{R}^n)$ associated with the translation group $\mathrm{Trans}(\mathbb{R}^n)$, and use corollary 2.2.13. The matrices W_i are in this case $W_i = I_n\, \partial_i$, $1 \leqslant i \leqslant n$. If we take the exponential of this module (that is the exponential of any of its elements) and apply it to any point of $\mathbb{R}^n$, we obtain an n-dimensional lattice in the Euclidean manifold $\mathbb{R}^n$; considering that the origin point o, with coordinates $u_o = 0 = (0; \ldots; 0)$ belongs to the lattice, we apply $\exp(\mathfrak{Z}_B^n)$ to this point, and obtain :

$$\Lambda = \exp(\mathfrak{Z}_B^n)\, u|_o = \{ B\,\lambda \mid \lambda = (\lambda_1; \ldots; \lambda_n) \in \mathbb{Z}^n \} , \tag{2.3.5}$$

where the matrix B defines the geometry, *i.e.* the shape of the lattice. The $\mathbb{Z}$-module $\mathfrak{Z}_B^n$ generates also a lattice in the tangent space $\mathrm{T}_o\mathbb{R}^n$ at the origin :

$$\Upsilon_o = \mathfrak{Z}_B^n\, u|_o = \{ B\,\lambda \mid \lambda = (\lambda_1; \ldots; \lambda_n) \in \mathbb{Z}^n \} , \tag{2.3.6}$$

which is the representation of the lattice Λ in $\mathrm{T}_o\mathbb{R}^n$. Corollary 2.2.13 shows that Υ_o can also be obtained by taking the tangent vector v at o of curves linearly parameterised between 0 and 1, linking the origin o to any node of Λ :

$$\begin{aligned} \gamma: \quad [0\,; 1] &\longrightarrow \mathbb{R}^n \\ t &\longmapsto \gamma(t) = B\,\lambda\,t \ , \end{aligned}$$

generated by the action of subsets of the one-parameter subgroups :

$$\begin{aligned} [0\,; 1] &\longrightarrow \mathrm{Trans}(M) \\ t &\longmapsto \exp(t\,Z) \ , \qquad Z \in \mathfrak{Z}_B^n \ , \end{aligned}$$
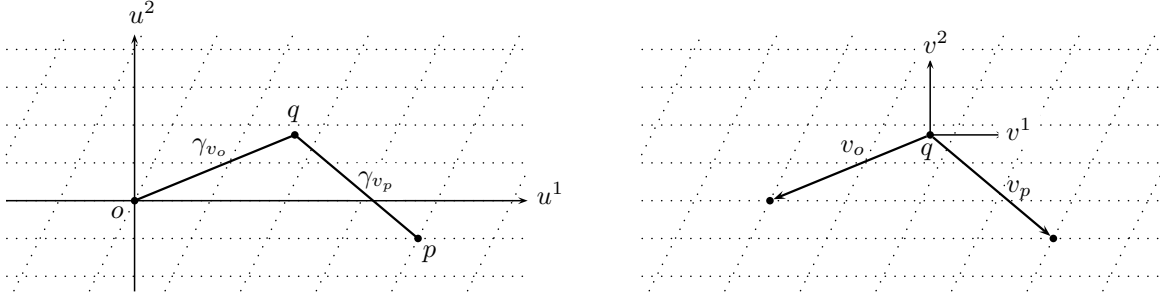
Figure 2.2: Example of a two dimensional periodic lattice viewed in the manifold $\mathbb{R}^2$ endowed with the natural (cartesian) coordinate system (left), and in its tangent space at q, $\mathrm{T}_q\mathbb{R}^2$ (right). Note that the appropriate crystallographic coordinate system (adapted to the shape of the lattice) could be used, the representation of the lattice in the tangent space at q would be exactly the same.

on the origin point o of $\mathbb{R}^n$. We effectively find :

$$v = \dot{\gamma}(0) = B\,\lambda \in \Upsilon_o \ .$$

All these calculations show that the Euclidean manifold $\mathbb{R}^n$ and its tangent space $\mathrm{T}_o\mathbb{R}^n$ have very close properties. Any figure, for instance the lattice Λ, has exactly the same shape in $\mathbb{R}^n$ as in $\mathrm{T}_o\mathbb{R}^n$.

The technique to obtain Υ_o based on the calculation of the tangent vectors of the curves $\gamma : t \mapsto B\,\lambda\,t$ can be used to define the concept of representation of a lattice $\Lambda \subset \mathbb{R}^n$ in any tangent space. Let :

$$\begin{aligned} \gamma : \quad [0\,;1] &\longrightarrow \quad \mathbb{R}^n \\ t &\longmapsto \quad \gamma(t) = u_q + (B\,\lambda - u_q)\,t \ . \end{aligned}$$

be the geodesic linearly parameterised between 0 and 1, linking the point q with coordinates u_q to any node of Λ. Its tangent vector at q is :

$$v = \dot{\gamma}(0) = B\,\lambda - u_q \ .$$

By analogy with Υ_o, the set of all tangent vectors v :

$$\Upsilon_q = \left\{ v = B\,\lambda - u_q \mid \lambda \in \mathbb{Z}^n \right\} \ . \tag{2.3.7}$$

is called *representation of Λ in $\mathrm{T}_q\mathbb{R}^n$*. It shares most features with Λ, therefore also with Υ_o : the pattern is also completely the same, it is just translated by $-u_q$, which is quite intuitive : the translation of $-u_q$ compensates for the fact that $\mathrm{T}_q\mathbb{R}^n$ is shifted from the tangent space at the origin of u_q (see figure 2.2).

As seen in chapter 1, an n-dimensional periodic crystal structure consists in a repetition in n dimensions of a unit cell, that is an n-dimensional parallelepiped composed of a certain number of atoms. Formally, such a structure can be given by the set :

$$\mathcal{S} = \left\{ u_\alpha + B\,\lambda \mid 1 \leqslant \alpha \leqslant \mu, \ \lambda \in \mathbb{Z}^n \right\} \ , \tag{2.3.8}$$

where μ is the number of atom in a unit cell, u_α are the coordinates (atomic position) of the atom α in a considered cell and B is the invertible matrix characterising the shape of the cell, hence the shape of the associated lattice $\{B\,\lambda \mid \lambda \in \mathbb{Z}^n\}$. All considerations previously done for Λ can be extended to $\mathcal{S}$: from the subset

$$\mathfrak{S} = \left\{ \sum_{j=1}^{n} s^j\,W_j \;\middle|\; s^j = u_\alpha{}^j + (B\,\lambda)^j,\; 1 \leqslant j \leqslant n,\; 1 \leqslant \alpha \leqslant \mu,\; \text{and } \lambda \in \mathbb{Z}^n \right\} \qquad (2.3.9)$$

of $\mathfrak{trans}(\mathbb{R}^n)$, we obtain the structure $\mathcal{S} = \exp(\mathfrak{S})\,u|_o = S$, as well as its representation $\mathcal{T}_o = \mathfrak{S}\,u|_o$ in the tangent space at o :

$$\mathcal{T}_o = \{u_\alpha + B\,\lambda \mid 1 \leqslant \alpha \leqslant \mu,\; \lambda \in \mathbb{Z}^n\} \;. \qquad (2.3.10)$$

This latter corresponds exactly to $\mathcal{S}$. The representation $\mathcal{T}_q$ of $\mathcal{S}$ in the tangent at any point q is :

$$\mathcal{T}_q = \{u_\alpha + B\,\lambda - u_q \mid 1 \leqslant \alpha \leqslant \mu,\; \lambda \in \mathbb{Z}^n\} \;; \qquad (2.3.11)$$

it corresponds to $\mathcal{T}_o$ translated by $-u_q$. At this point, one might wonder if these derivations are not just a more complicated way for describing known concepts : a structure $\mathcal{S} \subset \mathbb{R}^n$ is generated by a subset $\mathfrak{S} \subset \mathfrak{trans}(\mathbb{R}^n)$ which in fact corresponds to $\mathcal{S}$ itself (as $\mathfrak{trans}(\mathbb{R}^n) \cong \mathbb{R}^n$). However, this is not a vain effort, as the same procedure will be used for the description of modulated crystals.

2.3.2   Modulated Structures

As seen in the previous chapter, such structures are characterised by a basic (or average) structure (see expression 2.3.8), to which a *modulation* is applied. Formally, such a modulation can be seen as a one-to-one map $H = (h^1;\ \ldots;\ h^n)$ from $\mathbb{R}^n$ to itself, which can be written as $H = \mathrm{id} + \tilde{H}$, where $\tilde{H}$ is a periodic wave function : $\tilde{H}(u) \doteq \tilde{H}(\xi \cdot u)$, ξ being the wave vector, and $\tilde{H}(\xi \cdot u + T) = \tilde{H}(\xi \cdot u)$, for a $T \in \mathbb{R}_+^*$. H is one-to-one in order to avoid the possibility of finding two different atoms at the same position. Thus, we can think of $\mathbb{R}^n$ as an n-dimensional manifold M parameterised by H; M is included in $\mathbb{R}^n$ and $\mathbb{R}^n$ is included in M; H^{-1} is a curved coordinate system. Since $M \subset \mathbb{R}^n$, any $p \in M$ is also a point in $\mathbb{R}^n$, the position of which is then given by the n-tuple $\left(h^1(u_p);\ \ldots;\ h^n(u_p)\right)$. Note that this latter corresponds to the natural coordinates of p in $\mathbb{R}^n$ and not to the coordinates of p in M. To illustrate and clarify this point, we consider the example of the two-dimensional sphere $\mathbb{S}^2$ embedded in $\mathbb{R}^3$; any point p of $\mathbb{S}^2$, which is characterised by two numbers θ_p and φ_p (the latitude and longitude angles), is also a point in $\mathbb{R}^3$, the coordinates of which are $(\sin\theta_p\cos\varphi_p;\ \sin\theta_p\sin\varphi_p;\ \cos\theta_p)$.

For crystallographic applications, H is a periodic function of the position, smooth or only piecewise smooth in the case of *crenel* or *saw-tooth* shapes. This does not create a real problem, as any periodic function can be expanded in a Fourier series, hence it can be approximated by a smooth map.

Let M be an n-dimensional manifold M, parameterised by a one-to-one map $H : \mathbb{R}^n \to M$, $H = (h^1;\ \ldots,\ h^n)$, such that $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$. Two points q and p,

with coordinates $H(u_q) = \big(h^1(u_q); \ldots; h^n(u_q)\big)$ and $H(u_p) = \big(h^1(u_p); \ldots; h^n(u_p)\big)$ respectively, may be linked in M by a curve parameterised between 0 and 1 :

$$\gamma : \quad [0\,;\,1] \quad \longrightarrow \quad \mathbb{R}^n$$
$$t \quad \longmapsto \quad \gamma(t) = H\big(u_q + (u_p - u_q)\,t\big) \ ,$$

generated by the action of the subset of the one-parameter subgroup of translations :

$$[0\,;\,1] \quad \longrightarrow \quad \mathrm{Trans}(\mathbb{R}^n)$$
$$t \quad \longmapsto \quad I_n \exp\left(t \sum_{j=1}^{n} v^j\,\partial_j\right) \quad ,$$

where $v^j = u_p{}^j - u_q{}^j$, $1 \leqslant j \leqslant n$. Indeed :

$$I_n \exp\left(t \sum_{j=1}^{n} v^j\,\partial_j\right) H(u)\Big|_q = H(u_q + t\,v) \ ,$$

with $v = u_p - u_q$. When $t = 1$, $H(u_q + v) = H(u_p)$. The tangent vector of γ at q is :

$$\frac{\mathrm{d}\gamma(t)}{\mathrm{d}t}\bigg|_{t=0} = \dot{\gamma}(0) = \sum_{j=1}^{n} \frac{\partial H(u)}{\partial u^j}\bigg|_q (u_p{}^j - u_q{}^j) = \sum_{j=1}^{n} \frac{\partial H(u)}{\partial u^j}\bigg|_q v^j \doteq \tilde{v} \ ; \qquad (2.3.12\mathrm{a})$$

in components :

$$\tilde{v}^i = \sum_{j=1}^{n} \frac{\partial h^i(u)}{\partial u^j}\bigg|_q (u_p{}^j - u_q{}^j) \ ; \qquad (2.3.12\mathrm{b})$$

the point p, with coordinates $H(u_p)$ is represented in $\mathrm{T}_q M$ by the tip of the $\tilde{v}$ arrow. $\tilde{v}$ is then called the *representation of the point p in* $\mathrm{T}_q M$. In a compact form, it is noted $\tilde{v} = \mathrm{d}H_q(v)$, where $\mathrm{d}H_q$ is the differential map of H at q and is represented by the matrix $\left(\frac{\partial h^i}{\partial u^j}(q)\right)_{i,j=1}^{n}$. Note that the curve γ, which is in M, therefore also in $\mathbb{R}^n$, is not a straight line, hence not a geodesic. This does not create a problem; the important point is that there exists exactly one curve of the form of γ linking the two points q and p; this is the case, as H is one-to-one and as there exists exactly one straight line linking two points in $\mathbb{R}^n$. γ is the deformation of a geodesic in the Euclidean space, through H; it is the unique curve starting at q, generated by the curve $t \mapsto I_n \exp\left(\sum_{j=1}^{n} v^j\,\partial_j\right)$, $t \in [0\,;\,1]$. Thus, the ideas used in the definition of the exponential map may be generalised to other families of curves.

Let us consider the n-dimensional modulated lattice $\tilde{\Lambda}$ in M, corresponding to the deformation of the lattice Λ (see expression 2.3.5) through H :

$$\tilde{\Lambda} = \{H(B\,\lambda) \mid \lambda \in \mathbb{Z}^n\} \ .$$

Corollary 2.2.13 shows that $\tilde{\Lambda}$ is generated by the same module $\mathfrak{Z}_B^n$ (see expression 2.3.4) as in the case of Λ in the Euclidean manifold. Indeed, the action of $\exp(Z)$,

where $Z = \sum_{j=1}^{n} (B\,\lambda)^j\, W_j \in \mathfrak{Z}_B^n$, on the origin point o of M, with coordinates $H(u_o) = \left(h^1(u_o);\,\ldots;\,h^n(u_o)\right) = \left(h^1(0);\,\ldots;\,h^n(0)\right)$, is :

$$\exp\left(\sum_{j=1}^{n} (B\,\lambda)^j\, W_j\right) H(u)\Big|_o \;=\; I_n \exp\left(\sum_{j=1}^{n} (B\,\lambda)^j\, \partial_j\right) H(u)\Big|_o \;=\; H(B\,\lambda)\;,$$

where $\lambda \in \mathbb{Z}^n$. The module $\mathfrak{Z}_B^n$ also generates a lattice in the tangent space $\mathrm{T}_o M$ of M at the origin o :

$$\tilde{\Upsilon}_o \;=\; \mathfrak{Z}_B^n\, H(u)\big|_o \;=\; \{\Omega(0)\, B\,\lambda \mid \lambda \in \mathbb{Z}^n\}\;, \tag{2.3.13}$$

where $\Omega(0) \doteq \left(\frac{\partial h^i}{\partial u^j}(0)\right)_{i,j=1}^{n}$; $\tilde{\Upsilon}_o$ is the representation of the lattice $\tilde{\Lambda}$ in $\mathrm{T}_o M$. According to corollary 2.2.13, it can also be obtained by taking the curves :

$$\gamma:\quad \begin{aligned}[0\,;1] &\;\longrightarrow\; \mathbb{R}^n \\ t &\;\longmapsto\; \gamma(t) = H(B\,\lambda\, t)\;, \quad \lambda \in \mathbb{Z}^n\;,\end{aligned}$$

and calculating their tangent vector at o :

$$\dot{\gamma}(0) = \Omega(0)\, B\,\lambda\;.$$

Υ_o is a perfectly periodic lattice of translation, in the sense that it is an n-dimensional finite free $\mathbb{Z}$-module; it corresponds to the deformation of the lattice Λ through the matrix $\Omega(0)$.

To find the shape of $\tilde{\Lambda}$ in any tangent space, we follow the same path as in the Euclidean case. We consider the curves, generated by one-parameter subgroups of translations, linking the point q with coordinates $H(u_q) \in \mathbb{R}^n$ to any node of $\tilde{\Lambda}$:

$$\gamma:\quad \begin{aligned}[0\,;1] &\;\longrightarrow\; \mathbb{R}^n \\ t &\;\longmapsto\; \gamma(t) = H\big(u_q + (B\,\lambda - u_q)\,t\big)\;,\end{aligned}$$

and calculate their tangent vector at q :

$$\dot{\gamma}(0) = \Omega(u_q)\,(B\,\lambda - u_q)\;,$$

where $\Omega(u_q)$ is the matrix representation of the differential map $\mathrm{d}H_q$ of H. In components :

$$\dot{\gamma}^i(0) = \sum_{j=1}^{n} \frac{\partial h^i(u)}{\partial u^j}\bigg|_q (B\,\lambda - u_q)^j\;.$$

By analogy with $\tilde{\Upsilon}_0$, the set

$$\tilde{\Upsilon}_q = \{\Omega(u_q)\,(B\,\lambda - u_q) \mid \lambda \in \mathbb{Z}^n\}$$

is called *representation of* Λ *in* $\mathrm{T}_q M$. It corresponds to the lattice Λ distorted by the matrix $\Omega(u_q)$ and translated. These derivations show that a lattice Λ distorted by a function H recovers a linearity in the tangent spaces (see figure 2.3).
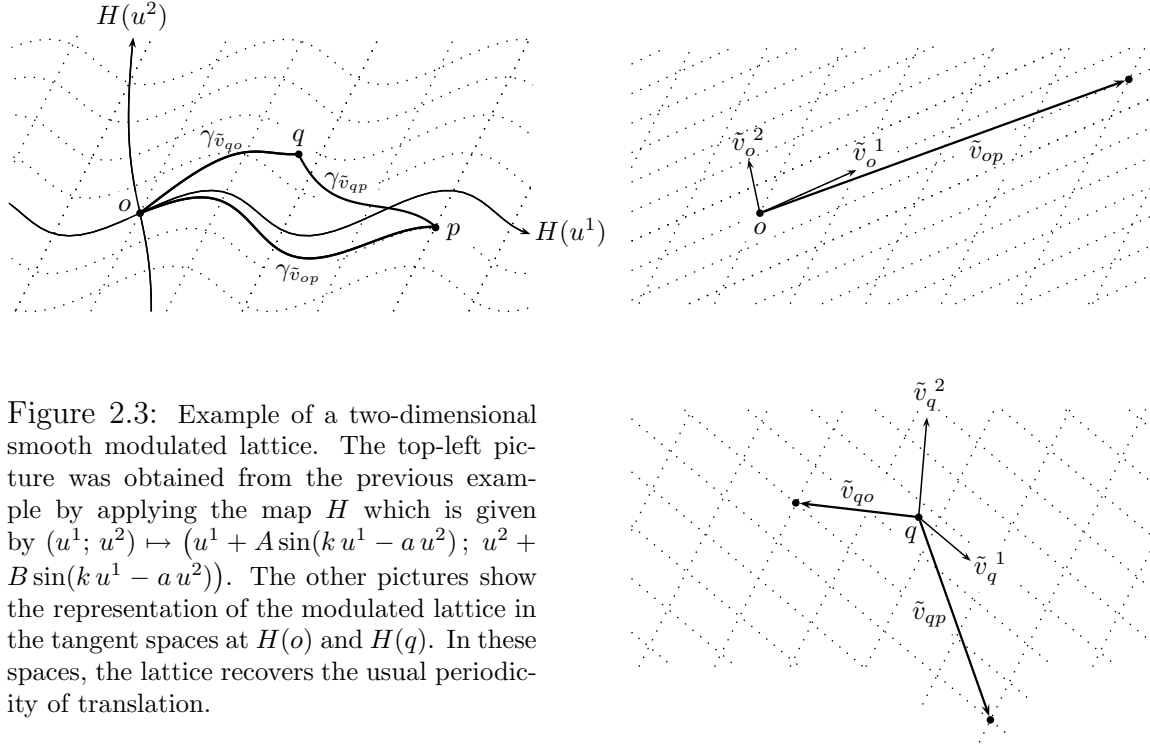
Figure 2.3: Example of a two-dimensional smooth modulated lattice. The top-left picture was obtained from the previous example by applying the map H which is given by $(u^1; u^2) \mapsto \left(u^1 + A\sin(k\,u^1 - a\,u^2);\ u^2 + B\sin(k\,u^1 - a\,u^2)\right)$. The other pictures show the representation of the modulated lattice in the tangent spaces at $H(o)$ and $H(q)$. In these spaces, the lattice recovers the usual periodicity of translation.

As mentioned at the beginning of this subsection, a modulated structure $\tilde{\mathcal{S}}$ is a distortion through the map H of an average structure $\mathcal{S}$, that is a structure in the Euclidean manifold (see expression 2.3.8). Formally :

$$\tilde{\mathcal{S}} = \{H(u_\alpha + B\,\lambda) \mid 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n\} \, , \qquad (2.3.14)$$

where u_α are the coordinates (atomic position) of the atom α in the unit cell of the average structure. According to corollary 2.2.13, $\tilde{\mathcal{S}}$ is generated by the same subset $\mathfrak{S}$ (see expression 2.3.9) as $\mathcal{S}$ in the Euclidean manifold. Indeed, the action of the exponential of an element of $\mathfrak{S}$ on the origin point o with coordinates $H(u_o) = H(0)$ is

$$\exp\left(\sum_{j=1}^{n}(u_\alpha{}^j + (B\,\lambda)^j)\,W_j\right) H(u)\big|_o \, = \, H(u_\alpha + B\,\lambda) \, ,$$

where $\lambda \in \mathbb{Z}^n$ and $1 \leqslant \alpha \leqslant \mu$. The representation $\tilde{\mathcal{T}}_o$ of $\tilde{\mathcal{S}}$ in the tangent space at the origin o is :

$$\tilde{\mathcal{T}}_o = \{\Omega(0)\,(u_\alpha + B\,\lambda) \mid 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n\} \, . \qquad (2.3.15)$$

Finally, the representation of $\tilde{\mathcal{S}}$ in the tangent space at any point q is :

$$\tilde{\mathcal{T}}_q = \{\Omega(u_q)\,(u_\alpha + B\,\lambda - u_q) \mid 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n\} \, . \qquad (2.3.16)$$

This last expression shows that the lattice $\{\Omega(u_q)\,B\,\Lambda \mid \lambda \in \mathbb{Z}^n\}$ associated with $\tilde{\mathcal{T}}_q$ is a finite free $\mathbb{Z}$-module, for any tangent point q.

2.3.3   Unified Description

The examples and illustrations presented in the past section show how corollary 2.2.13 is trivial in the Euclidean case and useful in the modulated case. The main result that should be kept in mind, is that the viewpoint adopted, based on manifold theory, provides a common playground for crystals, whether modulated or not :

2.3.1 Theorem : *Any crystal structure on a manifold M, parameterised by $H : \mathbb{R}^n \to M \subset \mathbb{R}^n$, and $\mathbb{R}^n \subset M$, is generated by a structure $\mathfrak{S} \subset \mathfrak{trans}(M)$, which can be written as :*

$$\mathfrak{S} = \left\{ \sum_{j=1}^n s^j\, W_j \;\middle|\; s^j = u_\alpha{}^j + (B\,\lambda)^j,\ 1 \leqslant j \leqslant n,\ 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n \right\}\ ,$$

With this structure is associated a lattice, the n-dimensional finite free $\mathbb{Z}$-module :

$$\mathfrak{Z}_B^n = \left\{ \sum_{j=1}^n (B\,\lambda)^j\, W_j \;\middle|\; \lambda \in \mathbb{Z}^n \right\}\ ,$$

where $B \in \mathrm{GL}_n(\mathbb{R})$. The modulated character is exclusively given by the geometrical properties of M, that is by the form of the parameterisation H. Thus, a unique structure $\mathfrak{S} \subset \mathfrak{trans}(M)$ generates a non-modulated structure, when H is the identity map, or a modulated one, when H is the sum of the identity map and a (periodic) wave function of the position.

2.3.2 Remark : Such a structure, whether modulated or not, containing μ atoms in a unit cell, is generated from one point, the origin o. This does not imply that all atoms have to be identical. This origin point can be seen as a pool containing all the atoms of the structure. Then, the set $\mathfrak{S}$ carries all atoms α (where $1 \leqslant \alpha \leqslant \mu$) to their positions $H(u_\alpha + B\,\lambda)$.

The last point of the theorem is very important because it shows that modulated structures should not be qualified as aperiodic. Of course, in the case where H is not the identity map, we cannot hope to have the same notion of periodicity as in a finite free $\mathbb{Z}$-module. But there is apparently no reason to consider vectors in manifolds; they are elements of tangent spaces and not of manifolds. Even in the Euclidean manifold, two points are linked by a curve, usually a straight line, and not by a vector. When this straight line is linearly parameterised between 0 and 1, the tip of its tangent vector at the starting point coincides with the end point. As the Euclidean manifold and its tangent spaces have very close geometrical properties, especially the tangent space at the origin, straight lines and vectors can be interchanged. If one does not stress these differences, vectors are used in inappropriate situations, for example for the description of atomic positions in modulated structures. Using the pertinent tools on appropriate spaces, the notion of aperiodic in modulated structures disappears completely. Two kinds of periodicity need to be distinguished : *vector periodicity*, which appears in any $\mathbb{Z}$-module, and *manifold* or *curve periodicity*, which appears in any lattice in a manifold M, generated by a finite free $\mathbb{Z}$-module in $\mathfrak{trans}(M)$. Thus, modulated structures have vector periodicity in any tangent space, and curve periodicity in the modulated manifold.

With all these considerations, we are in a position to give new definitions of concepts well-known in crystallography, namely the *point space* and the *associated vector space.*

2.3.3 Definition : The (so-called) n-dimensional *point space* is an n-dimensional (flat) manifold M such that $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$ parameterised by a one-to-one map $H : \mathbb{R}^n \to M$. If H is the identity map, this manifold is just $\mathbb{R}^n$ endowed with the natural coordinate system; hence it corresponds to the n-dimensional Euclidean space. When H is a periodic deformation of $\mathbb{R}^n$, the manifold corresponds to an n-dimensional modulated space in which modulated structures are described. This manifold corresponds mainly to $\mathbb{R}^n$, it is just endowed with a curved coordinate system (and not the natural one).

2.3.4 Definition : The (so-called) *associated vector space* is a tangent space of the manifold (the point space) at a particular point. Thus, as there is an infinity of tangent spaces, there is not only one associated vector space but an infinity. All these tangent spaces are isomorphic. In the Euclidean manifold, they just happen to be "geometrically equivalent" in the sense that they have all the same canonical (orthonormal) basis. In this case only, these tangent spaces have the same properties as the traditional associate vector space [Won02].

2.3.5 Remark : The fact that all tangent spaces of the Euclidean manifold have the same geometrical features is probably the reason why they are often merged and why one speaks about one and not several associated vector spaces.

2.4 Symmetry Operations

A unified description of crystals, whether modulated or not, is not fully consistent as long as a common formalism for symmetry operations is not obtained. The notion of symmetry operation of a structure has already been tackled in the previous chapter. However, a clear definition is essential. This will be done after discussing the concept of action of the Euclidean isometry group on a manifold M parameterised by a one-to-one map $H : \mathbb{R}^n \to M$.

2.4.1 The Euclidean Case

In the same way as in the theory of vector spaces, a linear isometry acts not only on the tip of the arrow but also on the whole vector, it is necessary to study how an isometry acts on whole curves and not on points only.

Recall that in the n-dimensional Euclidean space $\mathbb{R}^n$ endowed with the natural coordinate system, a straight line (geodesic), linearly parameterised between 0 and 1, and linking two points q and p, with coordinates $u_q = (u_q^1; \ldots; u_q^n)$ and $u_p = (u_p^1; \ldots; u_p^n)$ respectively, may be written as :

$$\gamma : \quad [0\,;1] \quad \longrightarrow \quad \mathbb{R}^n$$
$$t \quad \longmapsto \quad \gamma(t) = u_q + (u_p - u_q)\,t \;;$$

its tangent vector at q is $v \doteq u_p - u_q$. According to equation 2.1.15, a Euclidean isometry ϕ transforms any point of coordinates u into another of coordinates $u' = F\,u + s$, where $F \in \mathrm{O}_n(\mathbb{R})$ and $s \in \mathbb{R}$. Then, ϕ transforms any point of the above curve γ and therefore the whole curve into :

$$\gamma'(t) = F\,\gamma(t) + s = F\big(u_q + (u_p - u_q)\,t\big) + s \ .$$

The starting point of γ' is q', with coordinates $\gamma'(0) = F\,u_q + s$ and the end point is p' with coordinates $\gamma'(1) = F\,u_p + s$. The tangent vector of γ' at q' is :

$$\left.\frac{\mathrm{d}\gamma'(t)}{\mathrm{d}t}\right|_{t=0} = \dot{\gamma}'(0) = F\,(u_p - u_q) = F\,v \doteq v' \ .$$

This expression is particularly interesting because it expresses the action of the differential map $\mathrm{d}\phi_q$ of ϕ on vectors of the tangent space at q. Indeed, by definition, the differential map $\mathrm{d}\phi$, which is represented by the matrix F, carries vectors of the tangent space at a point, let us say q, to vectors of the tangent space at the point $\phi(q)$:

$$\begin{aligned} \mathrm{d}\phi_q : \mathrm{T}_q\mathbb{R}^n &\longrightarrow \mathrm{T}_{\phi(q)}\mathbb{R}^n \\ v &\longmapsto \mathrm{d}\phi_q(v) = v' \ . \end{aligned} \tag{2.4.1}$$

Thus, there exist two ways of determining the image of a point p through an isometry ϕ. The first, classical one, consists in applying the matrix and translation parts to u_p, the coordinates of p :

$$u'_p = F\,u_p + s \ .$$

The second one consists in considering the point p as the tip of a tangent vector v at q (it is then an element of the tangent space at q), and applying the differential map $\mathrm{d}\phi_q$ of ϕ to v, in order to obtain the vector v' in the tangent space at $\phi(q)$, the tip of which corresponds to a point in $\mathbb{R}^n$, namely $\phi(p)$.

   This alternative way is just a consequence of the Taylor development of ϕ. Indeed, as $\mathrm{d}\phi$ is represented by a constant matrix F (independent of the point in the manifold), its tangent application $\mathrm{d}(\mathrm{d}\phi)$ vanishes everywhere. Writing symbolically :

$$p = q + v \ , \quad v = p - q \tag{2.4.2}$$

for :

$$u_p = u_q + v \ , \quad v = (u_p - u_q) \ , \tag{2.4.3}$$

we have :

$$\phi(p) = \phi(q + v) = \phi(q) + \mathrm{d}\phi_q(v) \ . \tag{2.4.4}$$

In the general case, the left part of the above equation is a good approximation to the right side if v is small; but the bigger v is, the bigger remaining higher order terms are. In the present case, as ϕ corresponds to an affine map, there is no higher order terms and the above equation holds for every v.

   One might ask why such an elaborated procedure is derived to find the image of a point. Indeed, for a single point, it is needless to do so. However, by considering a large

Figure 2.4: Representations of an isometry ϕ which transforms a two-dimensional square lattice into itself. This corresponds to a rotation of angle $\frac{\pi}{2}$ around the point q of coordinates $\left(\frac{a}{2}\,;\frac{a}{2}\right)$. (1) shows the manifold representation of the four-fold axis isometry ϕ on the manifold. Two isometric triangles are drawn, the first one is composed of the points q, $\tilde{q}$ and p, the second one of their images. (2) and (2') show the tangent space representation of the four fold axis isometry. The "origin point" $\tilde{q}$ (which could also be the real origin point o) is carried to the "new origin point" $\phi(\tilde{q})$. The vectors $v_{\tilde{q}p}$ and $v_{\tilde{q}q}$ are carried to $v'_{\tilde{q}p}$ and $v'_{\tilde{q}q}$ respectively, through the differential map $\mathrm{d}\phi_{\tilde{q}}$. (3) and (3') indicate how convenient it is to choose the "origin point" $\tilde{q}$ at the fixed point q; to find the image of p, we only need to apply the tangent application $\mathrm{d}\phi_q$ to the vector v_{qp}.
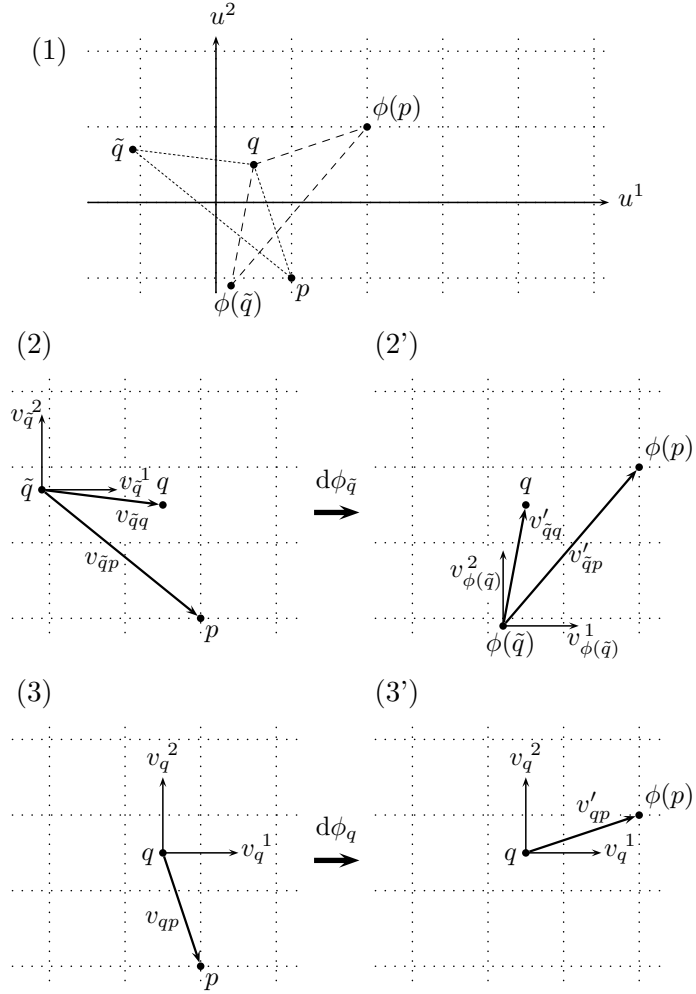
number of points, for instance nodes on an infinite lattice of translations (see expression 2.3.5), it becomes immediately useful. Taking one point q as an origin point and using the technique presented in the previous chapter (*i.e.* we link all nodes to q by straight lines linearly parameterised between 0 and 1, and calculate the tangent vectors $v_{q,B\lambda}$ of all these curves at q), we obtain the representation of this lattice in the tangent space $\mathrm{T}_q\mathbb{R}^n$ at q. The image of all these nodes through an isometry ϕ transforming the lattice into itself can be obtained just by calculating the image $\phi(q)$ of the point q and then by finding the image of the vectors $v_{q,B\lambda}$ through the tangent application $\mathrm{d}\phi_q$ (which is linear). This means that the translation part of the isometry appears only in the transformation of one point, the point q. The image of all others, the nodes in our case, are obtained by applying the linear map $\mathrm{d}\phi_q$. All these considerations are contained and summarised in expression 2.4.1.

Let us take the example of a two-dimensional square lattice

$$\Lambda^{\square} = \{a\,\lambda \mid \lambda \in \mathbb{Z}^2,\ a \in \mathbb{R}_+\}\ . \tag{2.4.5}$$

Among the isometries which transform this lattice into itself, there is the isometry ϕ which corresponds to a rotation of angle $\frac{\pi}{2}$ around the point q of coordinates $\left(\frac{a}{2}\,;\frac{a}{2}\right)$;

in the jargon of crystallography, it is called a four-fold point. In coordinates, ϕ can be written as :

$$\begin{pmatrix} u'^1 \\ u'^2 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} u^1 \\ u^2 \end{pmatrix} + \begin{pmatrix} a \\ 0 \end{pmatrix} \quad . \tag{2.4.6}$$

A node $(a\,\lambda^1;\, a\,\lambda^2)$ of this lattice becomes $(a\,(-\lambda^2+1);\, a\,\lambda^1)$. Let $\tilde{q}$ be an "origin point", with coordinates $(u_{\tilde{q}}^1;\, u_{\tilde{q}}^2)$. Any node of the lattice can be represented in the tangent space at $\tilde{q}$, by taking the tangent vector at $\tilde{q}$ of straight lines, linearly parameterised between 0 and 1, linking $\tilde{q}$ to the node under consideration. We obtain :

$$v = \begin{pmatrix} a\,\lambda^1 - u_{\tilde{q}}^1 \\ a\,\lambda^2 - u_{\tilde{q}}^2 \end{pmatrix} \quad .$$

By applying the rotation around q to the point $\tilde{q}$, we obtain its image $\phi(\tilde{q})$ with coordinates $(u_{\tilde{q}}'^1;\, u_{\tilde{q}}'^2) = (-u_{\tilde{q}}^2 + a\,;\, u_{\tilde{q}}^1)$. This image corresponds to a new "origin point". Applying next the matrix part of the rotation ϕ to the vectors v, we obtain their image :

$$v' = \begin{pmatrix} -a\,\lambda^2 + u_{\tilde{q}}^2 \\ a\,\lambda^1 - u_{\tilde{q}}^1 \end{pmatrix} \quad ,$$

which are elements of $\mathrm{T}_{\phi(\tilde{q})}\mathbb{R}^n$. These image vectors can be seen as tangent vectors at $\phi(\tilde{q})$ of straight lines, linearly parameterised between 0 and 1. The end points of these lines correspond to the tip of those tangent vectors. This means that by taking the coordinates of the point $\phi(\tilde{q})$ and adding the components of v', the coordinates of the image through ϕ of the lattice nodes are obtained; we have :

$$\begin{pmatrix} -u_{\tilde{q}}^2 + a \\ u_{\tilde{q}}^1 \end{pmatrix} + \begin{pmatrix} -a\,\lambda^2 + u_{\tilde{q}}^2 \\ a\,\lambda^1 - u_{\tilde{q}}^1 \end{pmatrix} = \begin{pmatrix} a\,(-\lambda^2 + 1) \\ a\,\lambda^1 \end{pmatrix} \quad ,$$

which is exactly the same result as if we directly apply ϕ to any node in the manifold (see figure 2.4). Note that the "origin point" $\tilde{q}$ can be any point of the manifold, in particular also the real origin point o of the coordinate system; ϕ then carries o to $\phi(o)$, the new "origin point".

2.4.2   The Importance of the Tangent Spaces

Should anybody wonder why so much importance is attached to the representation of points in tangent spaces of a manifold, the previous example of the square lattice gives a clear answer. In the tangent space at any point q, each point of the lattice $\Lambda^\square$ can be represented by a vector the image of which through an isometry ϕ is obtained just by the application of the differential map $\mathrm{d}\phi_q$ (which is represented by a constant matrix F). Note that the differential map is generally not an endomorphism of a vector space but a linear map between two tangent spaces. This means, in particular, that the translation part of an isometry does not completely : it appears in the image of the "origin point", vectors of a tangent space are carried to vectors of another tangent space. Realising this, manifold representation as well as that in tangent space can be equivalently used. Both contain the same information, it is just presented in a different way.

Note that in a special case, the differential map of an isometry ϕ can be an endomorphism, *i.e.* a linear map from a tangent space to itself. This happens when the isometry has a fixed point q, that is when $\phi(q) = q$. Considering the tangent space at this point and interpreting all other points of the Euclidean manifold as the tips of tangent vectors at q, we find that the differential map $\mathrm{d}\phi_q$ carries vectors of the tangent space at q to vectors of the tangent space at $\phi(q) = q$ (recall that $\mathrm{d}\phi_q : \mathrm{T}_q\mathbb{R}^n \to \mathrm{T}_q\mathbb{R}^n$). In the example of the square lattice $\Lambda^\square$ presented above, we observe indeed that in the tangent space at the rotation point q, a node of coordinates $(\lambda^1; \lambda^2)$ is given by the tip of the vector $\left(a\left(\lambda^1 - \frac{1}{2}\right); a\left(\lambda^2 - \frac{1}{2}\right)\right)$ in $\mathrm{T}_q\mathbb{R}^n$. Applying then the matrix part (representing the differential map) of ϕ, we obtain the vector $\left(-a\left(\lambda^2 - \frac{1}{2}\right); a\left(\lambda^1 - \frac{1}{2}\right)\right)$, also in $\mathrm{T}_q\mathbb{R}^n$, which corresponds, in the manifold, to the point of coordinates $\left(a\left(-\lambda^2 + 1\right); a\lambda^1\right)$.

2.4.3 The Modulated Case

As mentioned previously, an n-dimensional modulated structure is characterised by a periodic deformation of a basic structure $\mathcal{S}$ which lives in the n-dimensional Euclidean space. This deformation is mathematically described by the parameterisation $H : \mathbb{R}^n \to M$, where $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$. Let $\phi \in \mathrm{Isom}(\mathbb{R}^n)$ be a Euclidean isometry which transforms the basic structure into itself, that is $\phi(\mathcal{S}) = \mathcal{S}$. Then, for the corresponding modulated structure, which can be written as $\tilde{\mathcal{S}} = H(\mathcal{S})$, there exists a map $\tilde{\phi}$, defined by $\tilde{\phi} = H \circ \phi \circ H^{-1}$, which transforms $H(\mathcal{S})$ into itself. Indeed :

$$\tilde{\phi}(\tilde{\mathcal{S}}) = \tilde{\phi}\big(H(\mathcal{S})\big) = (H \circ \phi \circ H^{-1})\big(H(\mathcal{S})\big) = H\big(\phi(\mathcal{S})\big) = H(\mathcal{S}) = \tilde{\mathcal{S}} \ . \qquad (2.4.7)$$

Thus, the same map $\phi \in \mathrm{Isom}(\mathbb{R}^n)$ is at the origin of a transformation leaving a structure invariant; for the average structure $\mathcal{S}$, ϕ acts as $\phi(\mathcal{S})$, while for the modulated structure $\tilde{\mathcal{S}}$, ϕ is sandwiched between H and H^{-1} before it acts on $\tilde{\mathcal{S}}$.

Notice that such a form as $\tilde{\phi} = H \circ \phi \circ H^{-1}$ has already been seen previously, in the case where ϕ was a pure translation T (see remark 2.2.8); it is then not a surprise to meet it here again. The expression of $\tilde{\phi}$ is a simple consequence of the fact that $\tilde{\mathcal{S}}$ is generated by the same subset $\mathfrak{S} \in \mathfrak{trans}(\mathbb{R}^n)$ (see expression 2.3.9) as $\mathcal{S}$. As M is parameterised by one map $H : \mathbb{R}^n \to M$, $\mathfrak{trans}(\mathbb{R}^n) = \mathfrak{trans}(M)$. Since $\mathfrak{trans}(\mathbb{R}^n)$ is a vector space of dimension n, it is isomorphic to $\mathbb{R}^n$, seen as a vector space (see theorem 2.2.12). The isomorphism between these two spaces carries $\mathfrak{S} \in \mathfrak{trans}(\mathbb{R}^n)$ to a subset $\mathcal{S} \subset \mathbb{R}^n$, which can be written as :

$$\mathcal{S} = \left\{ s \mid s = u_\alpha + B\lambda, \ 1 \leqslant \alpha \leqslant \mu, \ \lambda \in \mathbb{Z}^n \right\} , \quad \text{with } B \in \mathrm{GL}_n(\mathbb{R}) \text{ fixed.} \qquad (2.4.8)$$

This set appears to be completely equal to $\mathcal{S}$. Formally, both are equal, their expression is exactly the same. There is, however, one difference, the geometrical aspect of the spaces in which the $\mathcal{S}$ and $\mathcal{S}$ are described : $\mathcal{S}$ is a structure in the n-dimensional Euclidean manifold $\mathbb{R}^n$ endowed with the natural coordinate system, while $\mathcal{S}$ is a set in $\mathbb{R}^n$, $\mathbb{R}^n$ being just an n-dimensional vector space in which no geometrical features have been defined and specified. If we consider this vector space as n copies of $\mathbb{R}$ which are declared as orthogonal between them, it can then be seen as the n-dimensional Euclidean manifold endowed with the natural coordinate system, and the n-tuples in $\mathcal{S}$ correspond

to natural coordinates. In this case, the isometry ϕ transforming the structure $\mathcal{S}$ into itself, also carries the set $\mathfrak{S}$ to itself. As long as we consider structures in the Euclidean space, one might think that our developments do not present any new feature, which is probably true. For modulated structures, however, an interesting result appears. Consider a point q in $\mathcal{S}$, with coordinates u_q. ϕ transforms it into another point q' of $\mathcal{S}$, with coordinates $u_{q'} = F\,u_q + r$, where $F \in O_n(\mathbb{R})$ and $r \in \mathbb{R}^n$ are the matrix and translation part of the expression of ϕ in the natural coordinate system. Thus the element $\sum_{j=1}^n u_q^j\,W_j \in \mathfrak{S}$ is transformed to $\sum_{j=1}^n u_{q'}^j\,W_j = \sum_{j=1}^n (F\,u_q + r)^j\,W_j \in \mathfrak{S}$. Through the exponential map, these two elements generate respectively $\exp\left(\sum_{j=1}^n u_q^j\,W_j\right)$ and $\exp\left(\sum_{j=1}^n (F\,u_q + r)^j\,W_j\right)$. Their action on the origin point o, with coordinates $H(0)$, of a manifold M, parameterised by the one-to-one map $H : \mathbb{R}^n \to M$, is :

$$\exp\left(\sum_{j=1}^n u_q^j\,W_j\right) H(0) \;=\; H(u_q)\;,$$

$$\exp\left(\sum_{j=1}^n (F\,u_q + r)^j\,W_j\right) H(0) \;=\; H(F\,u_q + r)\;.$$

We can then write $H(F\,u_q + r) = (H \circ \phi \circ H^{-1})\big(H(u_q)\big)$. As u_q and $F\,u_q + r$ are in $\mathcal{S}$, then $H(u_q)$ and $H(F\,u_q + r)$ are in $\tilde{\mathcal{S}}$. In conclusion, a Euclidean isometry ϕ transforming a structure $\mathcal{S}$ in the Euclidean manifold, is generated by an abstract map, which has the same matrix and translation part as ϕ, transforming $\mathfrak{S}$ into itself; in the case of a manifold M, parameterised by $H : \mathbb{R}^n \to M$, this abstract map generates the map $\tilde{\phi} = H \circ \phi \circ H^{-1}$.

As in the Euclidean case, let us study the action of $\tilde{\phi}$ on curves in the manifold M parameterised by the one-to-one map H. Recall that two points q and p in M, with coordinates $H(u_q)$ and $H(u_p)$ respectively, may be linked by a curve, parameterised between 0 and 1, in the following way :

$$\begin{aligned}\gamma : \quad [0\,;1] \quad &\longrightarrow \quad \mathbb{R}^n\\ t \quad &\longmapsto \quad \gamma(t) = H\big(u_q + (u_p - u_q)\,t\big)\;;\end{aligned}$$

its tangent vector at $H(q)$ is $\tilde{v} \doteq \sum_{j=1}^n \frac{\partial H}{\partial u^j}(q)\,(u_p - u_q)^j$, which can be written as $\tilde{v} = dH_q(u_p - u_q)$. Under the map $\tilde{\phi} = H \circ \phi \circ H^{-1}$, where ϕ is a Euclidean isometry with matrix and translation parts F and r, respectively, any point of the curve, therefore the whole curve becomes :

$$\gamma'(t) = H\big(F\,(u_q + (u_p - u_q)\,t) + r\big)$$

The starting point of γ' is q', with coordinates $\gamma'(0) = H(u_{q'}) = H(F\,u_q + r)$, and the end point is p', with coordinates $\gamma'(1) = H(u_{p'}) = H(F\,u_p + r)$. The tangent vector of γ' at q' is :

$$\left.\frac{d\gamma'(t)}{dt}\right|_{t=0} = \dot{\gamma}'(0) = \sum_{j=1}^n \frac{\partial H}{\partial u^j}(q')\,F\,(u_p - u_q) \doteq \tilde{v}'\;,$$

which can also be written as $\tilde{v}' = \mathrm{d}H_{\phi(q)}\big(\mathrm{d}\phi_q(u_p - u_q)\big)$. Note that $(u_p - u_q) = \Omega(q)^{-1}\,\tilde{v}$, where $\Omega(q)$ is the matrix representing $\mathrm{d}H_q$. Using the matrix notation, the expression above becomes :

$$\dot{\gamma}'(0) = \tilde{v}' = \Omega(q')\,F\,\Omega(q)^{-1}\,\tilde{v}\;,$$

where Ω and F are the matrix representations of $\mathrm{d}H$ and $\mathrm{d}\phi_q$ respectively. As in the Euclidean case, the image point p' of p can be obtained in two different ways. The first one consists in the application of $\tilde{\phi} \doteq H \circ \phi \circ H^{-1}$ to the point p, with coordinates $H(u_p)$:

$$H(u_p) \;\longmapsto\; \tilde{\phi}\big(H(u_p)\big) = H\big(\phi(u_p)\big)\;.$$

In the second one, we first find the vector in the tangent space at q, which corresponds to the tangent vector at q of the curve γ (parameterised between 0 and 1) linking q to p. We then apply the linear map $\Omega(q')\,F\,\Omega(q)^{-1}$, to finally obtain a vector in the tangent space at q', which is the tangent vector at q' of the curve γ' (parameterised between 0 and 1 in the same way) linking q' to p'. Note that the correspondance between curves (parameterised between 0 and 1) and their tangent vector at the starting point is unique. Thus, as in the Euclidean case, this second way of describing a symmetry operation contains as much information as the first one. This alternative is perhaps not so useful if we are interested in the image of one point only, but it is very practical when considering a large number of points, as in a lattice or a crystal structure. Moreover, it is also particularly friendly because the map $\tilde{\phi}$ is represented by a linear map : its differential map.

Let us illustrate this feature by the example of a two-dimensional modulated square lattice

$$\tilde{\Lambda}^{\square} = \{H(a\,\lambda) \mid \lambda \in \mathbb{Z}^2,\; a \in \mathbb{R}_+\}\;. \tag{2.4.10}$$

As seen before, the corresponding non-modulated lattice has, for instance, a four-fold point the coordinates of which are $\left(\frac{a}{2}\,;\,\frac{a}{2}\right)$. Since a rotation ϕ of $\frac{\pi}{2}$ around this point is given in coordinates by relation 2.4.6, $\tilde{\phi} = H \circ \phi \circ H^{-1}$ is a map which transforms $\tilde{\Lambda}^{\square}$ into itself. Let us now take an "origin point" $\tilde{q}$, with coordinates $H(u_{\tilde{q}})$. A curve, parameterised between 0 and 1, linking this point to any node of $\tilde{\Lambda}^{\square}$, may be written as $t \mapsto H(u_{\tilde{q}} + (a\,\lambda - u_{\tilde{q}})\,t) = \gamma(t)$. The components of its tangent vector at $\tilde{q}$ are :

$$\tilde{v} = \begin{pmatrix} \omega^1{}_1(\tilde{q}) & \omega^1{}_2(\tilde{q}) \\ \omega^2{}_1(\tilde{q}) & \omega^2{}_2(\tilde{q}) \end{pmatrix} \begin{pmatrix} a\,\lambda^1 - u_{\tilde{q}}^1 \\ a\,\lambda^2 - u_{\tilde{q}}^2 \end{pmatrix}\;,$$

where $\omega^i{}_j(\tilde{q}) = \frac{\partial h^i}{\partial u^j}\big|_{\tilde{q}}$, $1 \leqslant i,j \leqslant 2$, are the components of the matrix $\Omega(\tilde{q})$ representing $\mathrm{d}H_{\tilde{q}}$ ($\Omega(\tilde{q})$, sometimes also snoted $\Omega(u_{\tilde{q}})$). By applying $H \circ \phi \circ H^{-1}$ to $H(u_{\tilde{q}})$, we obtain the image $\tilde{q}'$ of $\tilde{q}$, with coordinates $H(u_{\tilde{q}'})$, which can be considered as a new "origin point". Taking the matrix part of ϕ, sandwiching it between $\Omega(\tilde{q}')$ and

Figure 2.5: Illustrations of a map $\tilde{\phi}$ which transforms a two-dimensional modulated square lattice into itself. The same four-fold axis as in the Euclidean space is taken and is sandwiched between H and H^{-1}, where H is the parameterisation of the manifold M in which the modulated lattice exists. The differential map of $\tilde{\phi}$ is $\mathrm{d}\tilde{\phi} = \mathrm{d}H_{q'} \circ \mathrm{d}\phi_q \circ (\mathrm{d}H_q)^{-1}$, where q' is the image of the point q through the map $\tilde{\phi}$; the matrix representation of this differential map can be written as $\Omega(\tilde{q}')\, F\, \Omega(\tilde{q})^{-1}$, where F and Ω are the matrices representing $\mathrm{d}\phi$ and $\mathrm{d}H$. As in the Euclidean example, (1) shows the action of the four-fold operation $\tilde{\phi}$ in the manifold. The two "triangles" $q\tilde{q}p$ and $q\tilde{q}'p'$, the edges of which are not straight lines but curves, are also represented. (2) and (2') show the tangent space representation of $\tilde{\phi}$. Note the difference of the shape of the lattice in $\mathrm{T}_{\tilde{q}}M$ and $\mathrm{T}_{\tilde{q}'}M$. (3) and (3') illustrate the situation in $\mathrm{T}_q M$; as q is a fixed point, the differential map $\mathrm{d}\tilde{\phi}_q$ is an endomorphism of the tangent space at q.
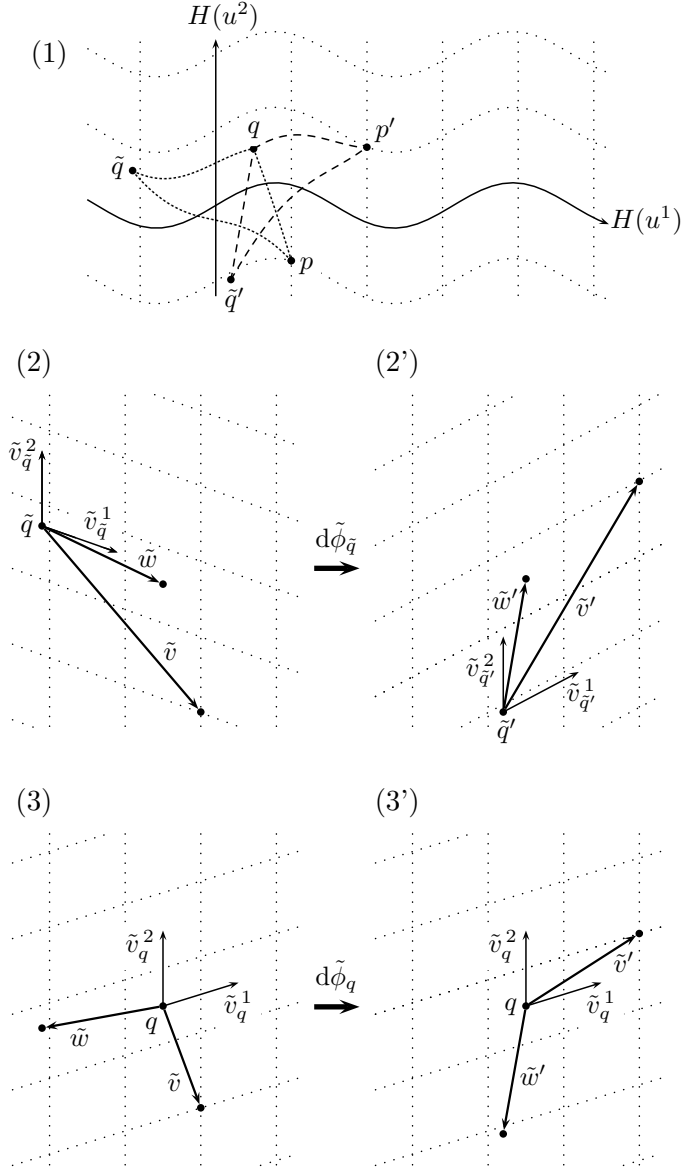
$\Omega(\tilde{q})^{-1}$, we obtain the matrix product :

$$\left(\begin{array}{cc} \omega^1{}_1(\tilde{q}') & \omega^1{}_2(\tilde{q}') \\ \omega^2{}_1(\tilde{q}') & \omega^2{}_2(\tilde{q}') \end{array} \right) \left(\begin{array}{cc} 0 & -1 \\ 1 & 0 \end{array} \right) \left(\begin{array}{cc} \varpi^1{}_1(\tilde{q}) & \varpi^1{}_2(\tilde{q}) \\ \varpi^2{}_1(\tilde{q}) & \varpi^2{}_2(\tilde{q}) \end{array} \right) ,$$

where $\varpi^i{}_j(\tilde{q})$, $1 \leqslant i, j \leqslant 2$ are the components of the matrix inverse to $\Omega(\tilde{q})$. This product of matrices transforms the vector $\tilde{v}$ of $\mathrm{T}_{\tilde{q}}M$ into the vector :

$$\tilde{v}' = \left(\begin{array}{cc} \omega^1{}_1(\tilde{q}') & \omega^1{}_2(\tilde{q}') \\ \omega^2{}_1(\tilde{q}') & \omega^2{}_2(\tilde{q}') \end{array} \right) \left(\begin{array}{c} -a\,\lambda^2 + u_{\tilde{q}}^2 \\ a\,\lambda^1 - u_{\tilde{q}}^1 \end{array} \right)$$

of $\mathrm{T}_{\tilde{q}'}M$, $\tilde{v}'$ being the tangent vector at $\tilde{q}'$ of the curve parameterised between 0 and 1 linking $\tilde{q}'$ to the image of the nodes of the modulated lattice (see figure 2.5).

2.4.4 Point and Space Group Operations

All the considerations and derivations done for the square lattice, whether modulated or not, can be extended to any crystal structure containing several atoms per unit cell. The description of a map transforming a structure into itself is the same in the Euclidean as well as in the modulated case, it is based on the action of the isometry group of $\mathbb{R}^n$ on a manifold M.

We are now in a position to define the concept of a crystallographic *symmetry operation*.

2.4.1 Definition : Let M be an n-dimensional manifold, such that $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$, parameterised by a (one-to-one) modulation function $H : \mathbb{R}^n \to M$ (see beginning of subsection 2.3.2). Let $\tilde{\mathcal{S}} \subset M$ be a structure generated by the subset $\mathfrak{S} \subset \mathfrak{trans}(\mathbb{R}^n)$ (see expression 2.3.9). A *symmetry operation* of the structure $\tilde{\mathcal{S}}$ is a map $\tilde{\phi} = H \circ \phi \circ H^{-1} : M \to M$, where $\phi \in \mathrm{Isom}(\mathbb{R}^n)$, which transforms $\tilde{\mathcal{S}}$ into itself.

2.4.2 Remark : Such a symmetry operation is generated by the isometry $\phi \in \mathrm{Isom}(\mathbb{R}^n)$ which can be seen as a symmetry operation of the structure $\mathcal{S}$ (see expression 2.4.8), provided that the vector space $\mathbb{R}^n$, in which $\mathcal{S}$ exists, be seen as the n-dimensional Euclidean space.

Thus, in the case where the parameterisation H is the identity map, M corresponds to the Euclidean space $\mathbb{R}^n$ and the isometry ϕ which transforms $\mathcal{S}$ into itself is equal to the symmetry operation of the structure $\mathcal{S} \in \mathbb{R}^n$. Note that linear maps are not considered as modulation functions, for otherwise it would imply that any lattice, whether modulated or not, could be obtained from the cubic one and then have the same symmetry operations!

2.4.3 Remark : The set of all symmetry operations of a structure, whether modulated or not, form a discrete group.

Let us return to the Euclidean case. A symmetry operation ϕ is represented by a matrix $F \in \mathrm{GL}_n(\mathbb{R})$ and a translation $r \in \mathbb{R}^n$ part, where $r \in \mathbb{R}^n$, and acts on points of $\mathbb{R}^n$ according to the formula 2.1.15 (s is just replaced here by r). The differential map $\mathrm{d}\phi$ of ϕ at any point is represented by the constant matrix F corresponding to the matrix part of ϕ. These two kinds of maps, as well as the very close relationship that exists between them, are reminiscent of concepts very well known in crystallography : *space group operations* and *point group operations*. Indeed, a space group operation is considered to be an affine transformation of the n-dimensional Euclidean space, that is the point space [Won02]. This is nothing else than an isometry on the Euclidean manifold. A point group operation associated with a space group operation is a linear map. This is just an isometry between two tangent spaces. Such a linear isometry is represented by a matrix corresponding to the linear part of the corresponding space group operation.

The main difference between the model based on differential geometry, and the traditional one lies in the fact that not only one but an infinite number of associated vector

spaces are considered. Moreover, all these considerations also hold in the modulated case. Thus, a more general definition of these fundamental concepts can be given.

2.4.4 Definition : A *space group operation* is a map acting in the point space, in the manifold, in which a (modulated) crystal structure $\tilde{\mathcal{S}}$ is described. In coordinates, such an operation may be written as $H \circ \phi \circ H^{-1}$, where H is the parameterisation of the manifold and ϕ an element of a discrete subgroup of the isometry group of Euclidean space. This subgroup contains all symmetry operations leaving the average crystal structure $\mathcal{S}$ invariant. Thus, $H \circ \phi \circ H^{-1}$ leaves the corresponding modulated structure invariant as well. If H is the identity map, the space (hence the crystal) is not modulated and $H \circ \phi \circ H^{-1} = \phi$.

2.4.5 Remark : Note that as all ϕ form a group, the set of all $H \circ \phi \circ H^{-1}$ also has the structure of a group. It is called *space group* when the dimension of M is 3, *plane* and *linear group* when the dimension of M is respectively 2 and 1.

2.4.6 Definition : A *point group operation* associated with a space group operation is a linear map between two tangent spaces of the manifold in which the crystal structure exists, whether modulated or not. It corresponds to the differential map of the space group operation. In matrix notation, such an operation may be written as $\Omega(q')\,F\,\Omega(q)^{-1}$, where Ω and F are the matrix representations of the differential maps $\mathrm{d}H$ and $\mathrm{d}\phi$, respectively. If H is the identity map, we just have $\Omega(q')\,F\,\Omega(q)^{-1} = F$.

2.4.7 Remark : As all elements ϕ leaving an average structure invariant form a group, so do the matrices F representing $\mathrm{d}\phi$, hence $\Omega(q')\,F\,\Omega(q)^{-1}$. The set of all point group operations is called *point group*.

Henceforth, a space group operation shall be also called *manifold representation* of a symmetry operation and a point group operation the *tangent space representation* of the symmetry operation. As in the Euclidean case, the tangent space representation contains as much information as the manifold one. The translation part appears in the image of the chosen tangent point.

Finally note that in all previous calculations, we did not insist too much on conditions for smoothness of H. However, modulated structures for which the modulation has a saw-tooth or crenel shape are not rare. In such cases, H is only piecewise smooth, the derivative of H does not exist everywhere. Nevertheless, all points where this latter is not defined form a set of zero measure and it is thus always possible to find points where the tangent space does exist. Moreover, as H is periodic, it can always been developed in a Fourier series, hence it can always be well approximated by a smooth function.

2.5   One-dimensional Modulated Structure

In order to illustrate the formalism developed in this chapter and compare it to the superspace model, nothing is better than to treat a concrete example of a modulated crystal. A one-dimensional structure will be considered, as the visualisation of figures

becomes difficult in three dimensions and impossible in more than three. Let $\mathcal{S}$ be one-dimensional non-modulated structure with linear group $p\bar{1}$, containing three atoms in a unit cell. According to the symmetry group, two of the three atoms are identical, one atom α and two atoms β are located in a unit cell. Their positions are, respectively :

$$u_\alpha = a\,\lambda \quad \text{and} \quad u_\beta = a\,\lambda \pm b\,, \quad \lambda \in \mathbb{Z}\,,$$

where $a \in \mathbb{R}_+$ is the unit cell parameter, and $0 < b < \frac{1}{2}\,a$. Consider further a sinusoidal modulation, such that the atoms α and β lie on the positions :

$$
\begin{aligned}
x_\alpha &= a\,\lambda + A_\alpha \sin(\xi\,a\,\lambda)\,, \\
x_{\beta_1} &= a\,\lambda + b + A_\beta \sin\big(\xi\,(a\,\lambda + b) + \varphi\big)\,, \\
x_{\beta_2} &= a\,\lambda - b + A_\beta \sin\big(\xi\,(a\,\lambda - b) - \varphi\big)\,,
\end{aligned}
$$

where $\xi, \varphi, A_\alpha, A_\beta \in \mathbb{R}$ (these parameters may in fact be chosen positive).

2.5.1   The Superspace Formalism

The modulated crystal is extended to a two-dimensional structure in a two-dimensional vector space endowed with the (non-orthonormal) basis $\{_2a_1;\ _2a_2\}$. With respect to an orthonormal basis, the components of $_2a_1$ and $_2a_2$ are :

$$_2a_1 = \begin{pmatrix} a \\ -\frac{\xi\,a}{\xi_\perp} \end{pmatrix}\,,$$

$$_2a_2 = \begin{pmatrix} 0 \\ -\frac{1}{\xi_\perp} \end{pmatrix}\,,$$

where $\xi_\perp$ is an arbitrary constant (see chapter 1, [JJLVdW02, SH01]). The first component of $_2a_1$ is the lattice parameter of the average structure which exists in the so-called *external* space, while the second one is $\xi\,a$ times the component of $_2a_2$ in the so called *internal* space (which is perpendicular to the external one). The two-dimensional structure is shown in figure 2.6. Its pattern is left invariant under rotations of angle π around the points
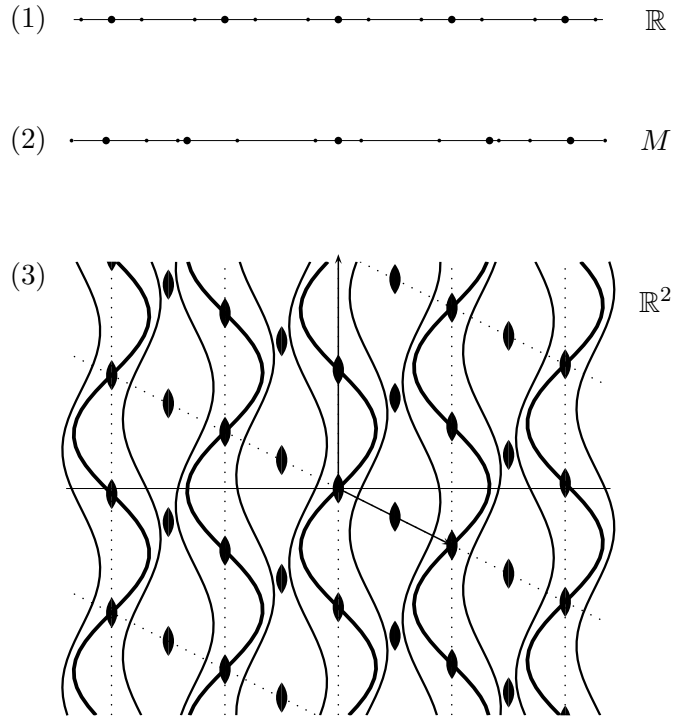

Figure 2.6: Superspace representation of a one-dimensionally modulated structure. (1) represents the average one-dimensional structure, (2) the corresponding modulated structure, and (3) shows the extension of the modulated structure in the two-dimensional superspace. Atoms are no longer points, but lines. The pattern is left invariant under rotations of angle π.

with coordinates $\left(\frac{n^1}{2}\,_2a_1;\ \frac{n^2}{2}\,_2a_2\right)$, where $n^1, n^2 \in \mathbb{Z}$. The matrix part of these symmetry operations is :

$$\left(\begin{array}{c|c} -1 & 0 \\ \hline 0 & -1 \end{array}\right) \quad ;$$

we see that the first component of this matrix corresponds to the inversion operation of the average structure.

2.5.2   Formalism Based on Differential Geometry

The whole one-dimensional space is modulated (distorted) by a map and the modulated structure $\tilde{\mathcal{S}}$ is *periodic* in this distorted space. To build this map, let us consider the bump function :

$$u \mapsto \varrho_s(u) = \begin{cases} \exp\left(1 - \frac{s^2}{s^2 - u^2}\right) & , \quad \text{when } |u| < s \\ 0 & , \quad \text{when } |u| \geqslant s \end{cases},$$

where $s \in \mathbb{R}_+$. It is smooth and reaches its maximum value 1 at $u = 0$. Taking this function, fixing $s = \frac{1}{2}b$, and shifting it in such a way that its maximum be at the position u_β of one of the atoms β (in the average structure), we obtain the function $u \mapsto \varrho(u - u_\beta)$, where :

$$\varrho_{\frac{b}{2}}(u - u_\beta) = \begin{cases} \exp\left(1 - \frac{b^2}{b^2 - 4\,(u - u_\beta)^2}\right) & , \quad |u - u_\beta| < \frac{b}{2} \\ 0 & , \quad |u - u_\beta| \geqslant \frac{b}{2} \end{cases}.$$

The one-to-one modulation map $h : \mathbb{R} \to \mathbb{R}$ is then simply given by :

$$\begin{aligned} u \mapsto h(u) = {} & \left(1 - \varrho_{\frac{b}{2}}(u - u_{\beta_1}) - \varrho_{\frac{b}{2}}(u - u_{\beta_2})\right) f(u) + \\ & + \varrho_{\frac{b}{2}}(u - u_{\beta_1})\, g(u) + \varrho_{\frac{b}{2}}(u - u_{\beta_2})\, \bar{g}(u) \;, \end{aligned}$$

where :

$$\begin{aligned} f(u) &= u + A_\alpha \sin(\xi\, u) \;, \\ g(u) &= u + A_\beta \sin(\xi\, u + \varphi) \;, \\ \bar{g}(u) &= u + A_\beta \sin(\xi\, u - \varphi) \;; \end{aligned}$$

u_{β_1} and u_{β_2} are the positions of the two atoms β. When $u = u_\alpha$, then $h(u_\alpha) = x_\alpha$, and when $u = u_{\beta_i}$, $h(u_{\beta_i}) = x_{\beta_i}$, $i = 1, 2$. Let p be any point of $\mathbb{R}$, with coordinate u_p, for instance such that $a - b < u_p < a$. Then, $\varrho_{\frac{b}{2}}(u_p - u_{\beta_1}) = 0$, hence :

$$h(u_p) = \left(1 - \varrho_{\frac{b}{2}}(u_p - u_{\beta_2})\right) f(u_p) + \varrho_{\frac{b}{2}}(u_p - u_{\beta_2})\, \bar{g}(u_p) \;,$$

and the differential map of h at this point is :

$$\begin{aligned} \mathrm{d}h_p = {} & -\mathrm{d}\varrho_{\frac{b}{2},p}\, f(u_p) + \left(1 - \varrho_{\frac{b}{2}}(u_p - u_{\beta_2})\right) \mathrm{d}f_p + \\ & + \mathrm{d}\varrho_{\frac{b}{2},p}\, \bar{g}(u_p) + \varrho_{\frac{b}{2}}(u_p - u_{\beta_2})\, \mathrm{d}\bar{g}_p \;, \end{aligned}$$

where :

$$\mathrm{d}\varrho_{\frac{b}{2},p} = -\frac{8\,b^2\,(u_p - u_{\beta_2})}{(b^2 - 4\,(u_p - u_{\beta_2})^2)^2}\,\exp\!\Big(1 - \tfrac{b^2}{b^2 - 4\,(u_p - u_{\beta_2})^2}\Big)\ ,$$

$$\mathrm{d}f_p = 1 + \xi\,A_\alpha\cos(\xi\,u_p)\ ,$$

$$\mathrm{d}\bar{g}_p = 1 + \xi\,A_\beta\cos(\xi\,u_p - \varphi)\ .$$

The positions of the atoms α and β of the one-dimensional modulated structure in the tangent space at the point of coordinates $h(u_p)$ (in the modulated space) are then :

$$\tilde{v}_\alpha = \Omega(u_p)\,(a\,\lambda - u_p)\ ,$$

$$\tilde{v}_\beta = \Omega(u_p)\,(a\,\lambda \pm b - u_p)\ ,$$

where $\Omega(u_p)$ is the 1×1 matrix representing $\mathrm{d}h_p$; in this case, it is just a number, which provides a magnitude reminding to a scale in tangent space. Thus, the structure in the tangent space has vector periodicity, as its associated lattice $a\,\mathbb{Z}$ is isomorphic to $\mathbb{Z}$ which is a finite free module.

Let ϕ be the Euclidean isometry given by $u \mapsto -u + 2\,a$, leaving the average structure $\mathcal{S}$ invariant. In the jargon of crystallography, ϕ is called *inversion operation*, and the point p (in the non-modulated space) with coordinate a is called *symmetry element*; it is a fixed point, that is $\phi(p) = p$. In the modulated structure, the corresponding operation is given by $\tilde{\phi}$: $h(u) \mapsto h(-u+2\,a)$. The point $h(a)$ is a fixed point and may be called symmetry element as well.

The symmetry operation $\tilde{\phi}$ also has a tangent space representation. The "origin" point $h(u_p)$ is transfered to a new "origin" point $h(-u_p+2\,a)$ through $\tilde{\phi}$, and $\mathrm{d}\tilde{\phi}$ carries tangent vectors at the point of coordinates $h(u_p)$ into tangent vectors at the point with coordinates $h(-u_p + 2\,a)$. Thus, the image of the vectors $\tilde{v}_\alpha$ and $\tilde{v}_\beta$ through $\mathrm{d}\tilde{\phi}_p$
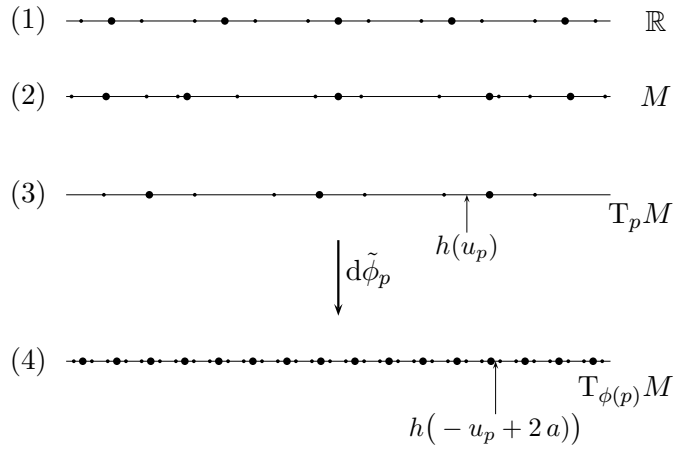
Figure 2.7: Representation of a one-dimensional modulated structure in tangent space. As in figure 2.6, (1) and (2) show the average and modulated structure respectively, (3) the representation of the modulated structure in the tangent space at the point of coordinates $h(u_p)$. After the application of the differential map $\mathrm{d}\tilde{\phi}_p$ (the "inversion" map), which carries vectors of the tangent space at the point of coordinates $h(u_p)$ into vectors of the tangent space at the image point of coordinates $h(-u_p+2\,a)$, we obtain (4), which corresponds exactly to the representation of the modulated structure in the tangent space at the image point.

is :

$$\tilde{v}'_\alpha = \mathrm{d}\tilde{\phi}_p(v_\alpha) = \Omega(-u_p + 2\,a)\,F\,\Omega(u_p)^{-1}\,\Omega(u_p)\,(a\,\lambda - u_p) =$$

$$= \Omega(-u_p + 2\,a)\,(-a\,\lambda + u_p)\;,$$

$$\tilde{v}'_\beta = \mathrm{d}\tilde{\phi}_p(v_\beta) = \Omega(-u_p + 2\,a)\,F\,\Omega(u_p)^{-1}\,\Omega(u_p)\,(a\,\lambda \pm b - u_p) =$$

$$= \Omega(-u_p + 2\,a)\,(-a\,\lambda \mp b + u_p)\;,$$

where $\Omega(-u_p + 2\,a)$ is the 1×1 matrix representing $\mathrm{d}h$ at the point of coordinates $h(-u_p + 2\,a)$ and $F = -1$ the 1×1 matrix representing $\mathrm{d}\phi$, the differential map of the (Euclidean) inversion operation ϕ. These vectors correspond exactly to the points in the manifold obtained by applying $\tilde{\phi}$ on the atomic positions in the modulated structure. Notice that in the case where $u_p = a$, $h(-u_p + 2\,a) = h(u_p)$ and $\mathrm{d}\tilde{\phi}_p$ is an endomorphism of the tangent space at the point of coordinates $h(u_p) = h(a)$ (see figure 2.7).

This example well illustrates that the symmetry of modulated structures can be described without adding dimensions, *i.e.* by remaining in the basic space. The notions of space group and point group operations hold for non-distorted, as well as for modulated crystals, without considering an additional dimension. In the formalism developed in this chapter, a symmetry operations is effectively not represented by an affine map any more. By using the tangent spaces, it can, however, always been represented by a linear map. Another difference between the superspace formalism and the model developed through this chapter is that the first imposes restrictions on the shape of the modulation and the modulation wave vector, whereas the second not. Indeed, in the previous one-dimensional example, the pattern in figure 2.6 can be left invariant under rotations of angle π only because the sinusoidal function is also left invariant under the same rotations. With the model based on differential geometry, the modulation can have any shape. Typically, the modulation applied to the square lattice in figure 2.5 is allowed in the formalism developed in this chapter, whereas it is forbidden in the superspace model; indeed, as the average square lattice is left invariant under a rotation of angle $\frac{\pi}{2}$, a modulation along one axis would necessarily imply a same modulation along the second one.

Nature seems to follow the constraints imposed by the superspace formalism. One can wonder if a modulated structure transgressing these rules will be once discovered. . .

Chapter 3

Structure in the Tangent Bundle of a Manifold

The tangent space representation of a structure has a substantial importance when dealing with symmetry operations. As the tangent point, that is the "origin" point of the considered tangent space, may be chosen arbitrarily, it appears legitimate to have the possibility to go from one tangent space to another one in a simple way.

Every coordinate system has a unique origin point, in that there is a unique point, the coordinates of which are all equal to zero. However, as seen in the previous chapter, for any tangent space, the corresponding tangent point can be considered as an "origin". Since there is an infinite number of points at which the manifold is smooth, there is an infinity of tangent points, *i.e.* an infinity of "origins", hence an infinity of representations of a structure in tangent spaces. When regrouped together, all these representation form a structure of double dimension in the tangent bundle of the considered manifold. Such a structure may easily be obtained by introducing an equivalence relation on the tangent bundle. Thanks to this relation, the representation of a structure in any tangent space can be found in a straightforward way. Moreover, a formalism in which symmetry operations no longer depend on the choice of an origin point is provided.

3.1 Fundamental Equivalence Relation on $\mathrm{T}M$

The motivation for defining an equivalence relation on the tangent bundle arises from the study of the manifold and tangent space representations of a lattice in Euclidean space. Recall that any two points q and p in the Euclidean space may be linked by a unique geodesic γ (straight line), *linearly* parameterised (*i.e.* with a constant velocity) between 0 and 1, such that $\gamma(0) = q$ and $\gamma(1) = p$. As shown in expression 2.3.3 of the previous chapter, the point p corresponds to the tip of the tangent vector v of γ at q. Let us focus on the point p; its position is independent of the starting point q and the curve linking q to p. Any straight line linearly parameterised between 0 and 1, the starting point of which is any point q and the endpoint p, is such that the tip of its tangent vector v at the starting point corresponds to p. The pairs $(q; v)$ and $(q'; v')$ may and will be considered as equivalent if and only if $\gamma_v(1) = \gamma_{v'}(1)$, where γ_v and $\gamma_{v'}$

are the straight lines (linearly parameterised between 0 and 1), the starting points of which are q and q' respectively, and the tangent vector of which are respectively v and v' at their starting point.

3.1.1   Equivalence Relation

Let us generalise the previous concepts to any n-dimensional manifold M, parameterised by the one-to-one map $H : \mathbb{R}^n \to M$, $H = (h^1; \ldots; h^n)$, such that $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$. Let q_1 and p be two points of M, with coordinates $H(u_{q_1})$ and $H(u_p)$. Recall that they can be linked by a curve γ parameterised between 0 and 1, and generated by the action of $\exp(t\,V_1)$ on $H(u_{q_1})$, where $t \in [0\,;\,1]$ and $V_1 = \sum_{j=1}^n v_1{}^j\, W_j$, $v_1{}^j = u_p{}^j - u_{q_1}{}^j$ and $W_j = I_n \partial_j$. The expression of this curve is :

$$
\begin{aligned}
\gamma : [0\,;\,1] &\longrightarrow M \\
t &\longmapsto \gamma(t) = H\big(u_{q_1} + (u_p - u_{q_1})\,t\big)\ .
\end{aligned}
$$

Its tangent vector at q_1 is $\tilde{v}_1$, the expression of which is $\tilde{v}_1 = \sum_{j=1}^n \frac{\partial H}{\partial u^j}(q_1)\,v_1{}^j = \Omega(u_{q_1})\,v_1$, where $v_1 = u_p - u_{q_1}$ and $\Omega = \big(\frac{\partial h^i}{\partial u^j}\big)_{i,j=1}^n$; in a compact notation, $\tilde{v}_1 = \mathrm{d}H_{q_1}(v_1)$. As γ is completely characterised by its starting point and tangent vector at the starting point, we shall write $\gamma_{\tilde{v}_1}$ instead of γ.

Taking another point q_2, with coordinates $H(u_{q_2})$, and following exactly the same path as above, we find another curve $\gamma_{\tilde{v}_2}$ linking q_2 to p, generated by the action of $\exp(t\,V_2)$ on $H(u_{q_2})$, where $t \in [0\,;\,1]$ and $V_2 = \sum_{j=1}^n v_2{}^j\, W_j$, $v_2{}^j = u_p{}^j - u_{q_2}{}^j$. It is given by :

$$
\begin{aligned}
\gamma_{\tilde{v}_2} : [0\,;\,1] &\longrightarrow M \\
t &\longmapsto \gamma_{\tilde{v}_2}(t) = H\big(u_{q_2} + (u_p - u_{q_2})\,t\big)\ ,
\end{aligned}
$$

and its tangent vector at q_2 is $\tilde{v}_2 = \sum_{j=1}^n \frac{\partial H}{\partial u^j}(q_2)\,v_2{}^j = \Omega(u_{q_2})\,v_2$, where $v_2 = u_p - u_{q_2}$; in a compact notation, $\tilde{v}_1 = \mathrm{d}H_{q_1}(v_1)$. Note that both curves, $\gamma_{\tilde{v}_1}$ and $\gamma_{\tilde{v}_2}$, have the same endpoint p with coordinates $H(u_p)$. Let us then introduce a relation $\sim$ as follows.

3.1.1 Definition : Let M be a manifold parameterised by the one-to-one map $H : \mathbb{R}^n \to M$, such that $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$. Let q_1 and q_2 be two points of M, with coordinates $H(u_{q_1})$ and $H(u_{q_2})$ respectively. We define a relation $\sim$ on the tangent bundle of M as follows :

$$
\big(H(u_{q_1})\,;\,\tilde{v}_1\big) \sim \big(H(u_{q_2})\,;\,\tilde{v}_2\big) \quad \Leftrightarrow \quad \gamma_{\tilde{v}_1}(1) = H(u_p) = \gamma_{\tilde{v}_2}(1)\ ,
$$

where $p \in M$ is a point with coordinates $H(u_p)$, which corresponds to the same endpoint of the curves $\gamma_{\tilde{v}_1}$ and $\gamma_{\tilde{v}_2}$, these curves being characterised by the starting point q_1 and q_2 respectively, and a tangent vector at their starting point $\tilde{v}_1$ and $\tilde{v}_2$, respectively.

3.1.2 Lemma : *The relation $\sim$, as defined above, is an equivalence relation on the tangent bundle* $\mathrm{T}M$ *of the manifold M.*

Indeed, $\sim$ is evidently reflexive and symmetric. To show the transitivity, we consider three couples $\big(H(u_{q_1})\,;\,\tilde{v}_1\big)$, $\big(H(u_{q_2})\,;\,\tilde{v}_2\big)$ and $\big(H(u_{q_3})\,;\,\tilde{v}_3\big)$ (the foots of $\tilde{v}_1$, $\tilde{v}_2$, $\tilde{v}_3$ being respectively on the points of coordinates $H(u_{q_1})$, $H(u_{q_2})$, $H(u_{q_3})$), such that $\big(H(u_{q_1})\,;\,\tilde{v}_1\big) \sim \big(H(u_{q_2})\,;\,\tilde{v}_2\big)$ and $\big(H(u_{q_2})\,;\,\tilde{v}_2\big) \sim \big(H(u_{q_3})\,;\,\tilde{v}_3\big)$. This means that $\gamma_{\tilde{v}_1}(1) = \gamma_{\tilde{v}_2}(1)$ and $\gamma_{\tilde{v}_2}(1) = \gamma_{\tilde{v}_3}(1)$, where $\gamma_{\tilde{v}_\alpha}$, $1 \leqslant \alpha \leqslant 3$, are curves the expressions of which are :

$$\begin{aligned} \gamma_{\tilde{v}_\alpha} : [0\,;\,1] &\longrightarrow M \\ t &\longmapsto \gamma_{\tilde{v}_\alpha}(t) = H\big(u_{q_\alpha} + (u_p - u_{q_\alpha})\,t\big)\ , \end{aligned}$$

Thus, $\gamma_{\tilde{v}_1}(1) = \gamma_{\tilde{v}_3}(1)$, hence $\big(H(u_{q_1})\,;\,\tilde{v}_1\big) \sim \big(H(u_{q_3})\,;\,\tilde{v}_3\big)$. $\blacksquare$

3.1.3 Remark : Any element of the tangent bundle of the manifold M (parameterised by $H : \mathbb{R}^n \to M$) can be written as a pair $\big(H(u)\,;\,\tilde{v}\big)$, where $H(u)$ and $\tilde{v}$ can both be written as n-tuples $\big(h^1(u);\,\ldots;\,h^n(u)\big)$ and $(\tilde{v}^1;\,\ldots;\,\tilde{v}^n)$ respectively. This shows that a one-to-one correspondance between the tangent bundle TM of M and the space $\mathbb{R}^n \times \mathbb{R}^n = \mathbb{R}^{2n}$ exists; we can therefore think of TM as $\mathbb{R}^n \times \mathbb{R}^n$.

3.1.2 Equivalence Class

Let $p \in M$ be a point with coordinates $H(u_p)$; by the natural immersion map $\iota : M \to$ TM, it can be seen as a point in the tangent bundle TM, the coordinate of which are $\big(H(u_p)\,;\,0\big)$. Let :

$$\begin{aligned} \gamma : [0\,;\,1] &\longrightarrow M \\ t &\longmapsto \gamma(t) = H\big(u_p + (1-t)\,w\big) \end{aligned}$$

be the curve linking the point of coordinates $\gamma(0) = H(u_p + w)$ to $H(u_p)$. Note that as w is any element of $\mathbb{R}^n$, then $\gamma(0)$ is any point in M (because H is one-to-one). The tangent vector of this curve at $t = 0$, *i.e.* at the point of coordinates $H(u_p + w)$, is :

$$\tilde{v} \doteqdot \dot{\gamma}(0) = -\sum_{j=1}^{n} \frac{\partial H}{\partial u^j}(u_p + w)\,w^j = -\Omega(u_p + w)\,w\ ,$$

where Ω is the matrix representing the differential map dH. According to the $\sim$ equivalence relation, all elements of TM which can be written as $\big(H(u_p + w)\,;\,-\Omega(u_p + w)\,w\big)$, where $w \in \mathbb{R}^n$ are equivalent and can be regrouped in a so-called *equivalent class*. To this class belongs also the element $\big(H(u_p)\,;\,0\big)$. The class can then be called *equivalence class of* $\big(H(u_p)\,;\,0\big)$, and may be written as :

$$\big[\big(H(u_p)\,;\,0\big)\big]_\sim \doteqdot \big(H(u_p + w)\,;\,-\Omega(u_p + w)\,w\big)\ , \quad \text{where } w \in \mathbb{R}^n\ .$$

$\big(H(u_p)\,;\,0\big)$ is called *representative* of the equivalence class. This representative is not unique; each point of the class may be a representative, for instance $\big(H(0)\,;\,\Omega(0)\,u_p\big)$ (when $w = u_p$). The same equivalence class may also be described from this other point :

$$\big[\big(H(u_p)\,;\,0\big)\big]_\sim = \big[\big(H(0)\,;\,\Omega(0)\,u_p\big)\big]_\sim = \big(H(\bar{w})\,;\,\Omega(\bar{w})(u_p - \bar{w})\big)\ , \quad \text{where } \bar{w} \in \mathbb{R}^n\ .$$

3.1.4 Definition : The equivalence class $\left[\left(H(u_p)\,;\,0\right)\right]_\sim$ is called *tangent bundle representation* of the point p.

3.1.5 Lemma : *The equivalence classes of $\sim$ are disjoint if H is a diffeomorphism.*

Indeed, let us consider two points in $\mathrm{T}M$ the coordinates of which are $\left(H(u_{p_1})\,;\,0\right)$ and $\left(H(u_{p_2})\,;\,0\right)$. Their equivalence class is respectively :

$$\left(H(u_{p_1} + w_1)\,;\,-\Omega(u_{p_1} + w_1)\,w_1\right) \quad,$$
$$\left(H(u_{p_2} + w_2)\,;\,-\Omega(u_{p_2} + w_2)\,w_2\right) \quad,$$

where $w_1, w_2 \in \mathbb{R}^n$ are two parameters. Consider the point $\left(H(u_q)\,;\,\tilde{v}_q\right)$ and suppose it belongs to both classes. This means that there exists $\bar{w}_1, \bar{w}_2 \in \mathbb{R}^n$ such that :

$$\left(H(u_q)\,;\,v_q\right) \;=\; \left(H(u_{p_1} + \bar{w}_1)\,;\,-\Omega(u_{p_1} + \bar{w}_1)\,\bar{w}_1\right)\,,$$
$$\left(H(u_q)\,;\,v_q\right) \;=\; \left(H(u_{p_2} + \bar{w}_2)\,;\,-\Omega(u_{p_2} + \bar{w}_2)\,\bar{w}_2\right)\,.$$

Since H is a diffeomorphism, H is bijective and Ω, which represents $\mathrm{d}H$, is a field of maximal rank matrices. So, H^{-1} and Ω^{-1} exist everywhere. Then, $H(u_{p_1} + \bar{w}_1) = H(u_q) = H(u_{p_2} + \bar{w}_2)$ implies that $u_{p_1} + \bar{w}_1 = u_q = u_{p_2} + \bar{w}_2$, hence :

$$\left(H(u_q)\,;\,v_q\right) \;=\; \left(H(u_q)\,;\,-\Omega(u_q)\,(u_q - u_{p_1})\right)\,,$$
$$\left(H(u_q)\,;\,v_q\right) \;=\; \left(H(u_q)\,;\,-\Omega(u_q)\,(u_q - u_{p_2})\right)\,.$$

From these equalities, we obtain $\Omega(u_q)\,(u_q - u_{p_1}) = \Omega(u_q)\,(u_q - u_{p_2})$, hence $u_q - u_{p_1} = u_q - u_{p_2}$. Thus, $u_{p_1} = u_{p_2}$ and $H(u_{p_1}) = H(u_{p_2})$; the two equivalence classes are therefore a single one.   ∎

3.1.6 Remark : Note that for crystallographic applications, H is a one-to-one map, which is only piecewise smooth, and the inverse of which is also piecewise smooth. This does not cause any difficulty, as it might always be well approximated by a diffeomorphism. Indeed, as H is a periodic wave function of the position, it can be developed in a Fourier series and approximated by a smooth map, when taking a finite number of terms.

3.1.3   The Euclidean Case

Let $\mathbb{R}^n$ be the n-dimensional Euclidean manifold endowed with the natural coordinate system $u = (u^1;\,\ldots;\,u^n)$. The equivalence relation on the tangent bundle defined above becomes very intuitive in this case (see figure 3.1) . Indeed, recall that in the Euclidean case, the end point of a straight line (a geodesic) linking two points q and p, and linearly parameterised between 0 and 1, corresponds to the tip of the tangent vector v of this geodesic at q (and the components of v correspond to the components of the vector in $\mathsf{trans}(\mathbb{R}^n)$ which generates this curve). Then, the relation :

$$(u_{q_1};\,v_1) \sim (u_{q_2};\,v_2) \quad \Leftrightarrow \quad \gamma_{v_1} = u_p = \gamma_{v_2}$$

Figure 3.1: Illustration of the equivalence relation on the tangent bundle of a manifold in the case of the two-dimensional Euclidean manifold. Two couples $(u_{q_1}; v_1)$ and $(u_{q_2}; v_2)$ are equivalent if and only if the tip of v_1 is at the same point as the tip of v_2. The couple $(u_{q_3}; v_3)$ is not equivalent to the two previous couples because the tip of v_3 is not at p.
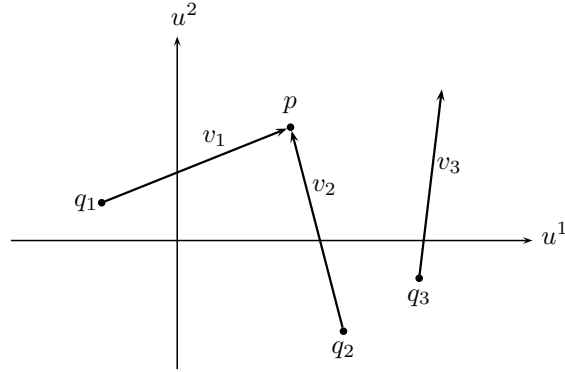
may be written as :

$$(u_{q_1};\, v_1) \sim (u_{q_2};\, v_2) \quad \Leftrightarrow \quad u_{q_1} + v_1 = u_{q_2} + v_2 \ .$$

This means that two points q_1 and q_2, with coordinates u_{q_1} and u_{q_2}, are related if the tip of the vectors v_1, with foot at q_1, and v_2, with foot at q_2, is at the same point.

The equivalence class of a point $(u_p; 0)$ in the tangent bundle of the Euclidean manifold is given by :

$$[(u_p; 0)]_\sim = (u_p + w\,;\, -w) \ \ ,$$

where $w \in \mathbb{R}^n$. From this expression, we see that the point p, the coordinates of which in the Euclidean space are u_p, is represented by the vector $-w = u_p - u_q$ in the tangent space at $u_q \doteq u_p + w$. According to definition 3.1.4, the equivalence class of $(u_p; 0)$ is the tangent bundle representation of the point p.

As an example, let us find the tangent bundle representation of a periodic lattice $\Lambda = \{B\,\lambda \mid \lambda \in \mathbb{Z}^n\}$, for a $B \in \mathrm{GL}_n(\mathbb{R})$, in the n-dimensional Euclidean space $\mathbb{R}^n$ (see also expression 2.3.5). As each tangent space of $\mathbb{R}^n$, seen as the Euclidean manifold endowed with the natural (cartesian) coordinate system, corresponds to $\mathbb{R}^n$, seen as the vector space $\mathbb{R}^n$ endowed with the canonical orthonormal basis, the tangent bundle of this manifold is $\mathbb{R}^n \times \mathbb{R}^n = \mathbb{R}^{2n}$. Each point $B\,\lambda \in \Lambda$ may be seen as an element of this tangent bundle and written as the pair $(B\,\lambda; 0)$. Its equivalence class (the tangent bundle representation) is then :

$$[(B\,\lambda\,;\, 0)]_\sim = (B\,\lambda + w_\lambda\,;\, -w_\lambda) \ , \quad \text{where} \ \ w_\lambda \in \mathbb{R}^n \ .$$

The equivalence classes of all nodes of Λ form a set :

$$\Xi = \{(B\,\lambda + w_\lambda\,;\, -w_\lambda) \mid w_\lambda \in \mathbb{R}^n, \lambda \in \mathbb{Z}^n\} \ ,$$

called *tangent bundle representation of* Λ. If for each $\lambda \in \mathbb{Z}^n$, we choose $w_\lambda = -B\,\lambda$, we obtain representatives of each class $[(B\,\lambda\,;\, 0)]_\sim$ which all belong to the same tangent space at the origin :

$$(0\,;\, B\,\lambda) \ \ , \quad \lambda \in \mathbb{Z}^n \ ;$$

The set of all these points corresponds to the representation of the lattice Λ in the tangent space at the origin (see expression 2.3.6). More generally, if we choose $w_\lambda = u_q - B\,\lambda$,

Figure 3.2: Representation of a one-dimensional periodic lattice in the tangent bundle $\mathbb{R}^2$ of the one-dimensional Euclidean manifold $\mathbb{R}$. A "vertical" cut through any point q, corresponds to the representation of the lattice in the tangent space at q.

where u_q are the coordinates of a point q, all representatives of each equivalence class belong to the same tangent space at q :

$$(u_q \,;\, -u_q + B\,\lambda) \,, \quad \lambda \in \mathbb{Z}^n \,;$$

the set of all these points form the representation of Λ in the tangent space at the chosen point q (see expression 2.3.7). Figure 3.2 shows the case of a one-dimensional periodic lattice. Equivalence classes of each node are straight lines of slope -1 and going through the corresponding point.

3.1.4   The Modulated Case

In any non-Euclidean case, the equivalence relation $\sim$ is a bit less intuitive because the tip of the tangent vector at the starting point of a curve parameterised between 0 and 1 does not coincide with its endpoint (see figure 3.3). However, it is not less useful, as it provides the representation of a point in any tangent space, as well as the connection between them and also the manifold.

Let M be a manifold parameterised by the one-to-one map $H : \mathbb{R}^n \to M$, such that $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$. The equivalence class of a point p with coordinates $H(u_p)$, seen as a point of coordinates $\big(H(u_p)\,;\, o\big)$ in the tangent bundle of M, is :

$$\big[\big(H(u_p)\,;\, 0\big)\big]_\sim = \big(H(u_p + w)\,;\, -\Omega(u_p + w)\, w\big) \,, \quad w \in \mathbb{R}^n \,,$$

where Ω is the matrix representing $\mathrm{d}H$. With this expression, we immediately see that the point p, the coordinates of which in the manifold are $H(u_p)$, is represented by the vector $-\Omega(u_p + w)\, w = \Omega(u_q)\,(u_p - u_q)$ in the tangent space at $H(u_q) \doteqdot H(u_p + w)$.

As an example, let us find the tangent bundle representation of a modulated lattice $\tilde{\Lambda} = \{H(B\,\lambda) \mid \lambda \in \mathbb{Z}^n\}$, where $B \in \mathrm{GL}_n(\mathbb{R})\}$ and $H : \mathbb{R}^n \to \mathbb{R}^n$ is the one-to-one map which defines the modulation (see also expression 2.3.2). Each point $H(B\,\lambda)$ of $\tilde{\Lambda}$ may be written as an element $\big(H(B\,\lambda)\,;\, 0\big)$ of the tangent bundle of the manifold. Its tangent space representation (equivalence class) is then :

$$\big[\big(H(B\,\lambda)\,;\, 0\big)\big]_\sim = \big(H(B\,\lambda + w_\lambda)\,;\, -\Omega(B\,\lambda + w_\lambda)\, w_\lambda\big) \,,$$

where $w_\lambda \in \mathbb{R}^n$. The equivalence classes of all nodes form a set :

$$\tilde{\Xi} = \big\{\big(H(B\,\lambda + w_\lambda)\,;\, -\Omega(B\,\lambda + w_\lambda)\, w_\lambda\big) \mid w_\lambda \in \mathbb{R}^n, \lambda \in \mathbb{Z}^n\big\} \,,$$
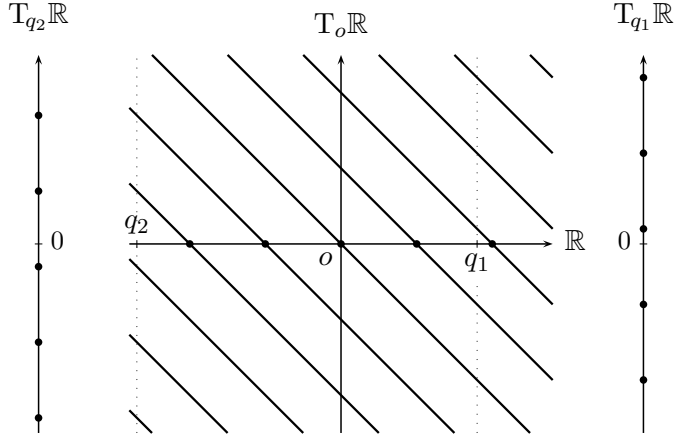
Figure 3.3: Illustration of the equivalence relation on the tangent bundle of a manifold in the modulated case (modulated manifold). Two couples $\left(H(u_{q_1})\,;\,\tilde{v}_1\right)$ and $\left(H(u_{q_2})\,;\,\tilde{v}_2\right)$ are equivalent if and only if the curves γ_{v_1} and γ_{v_2}, associated to the vectors $\tilde{v}_1$ and $\tilde{v}_2$ respectively, have the same end point p, with coordinates $H(u_p)$. The couple $\left(H(u_{q_3})\,;\,\tilde{v}_3\right)$ is not equivalent to the two previous couples because the end point of the curve γ_{v_3} associated to $\tilde{v}_3$ does not correspond to p.
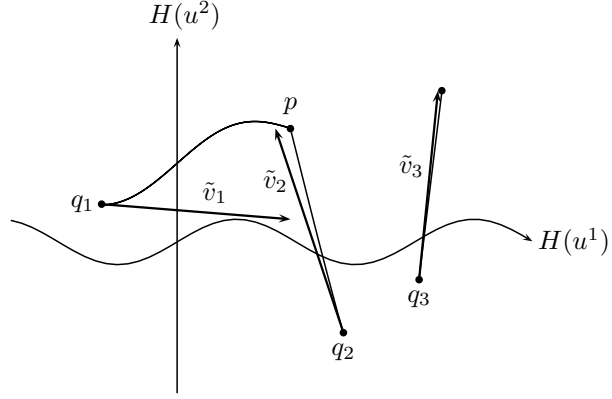
called *tangent bundle representation of the lattice* $\tilde{\Lambda}$. Choosing for each $\lambda \in \mathbb{Z}^n$, $w_\lambda = u_q - B\,\lambda$, we obtain representatives of each class which all belong to the same tangent space at the point q with coordinates $H(u_q)$:

$$\left(H(u_q)\,;\,\Omega(u_q)\,(-u_q + B\,\lambda)\right)\,,\quad \lambda \in \mathbb{Z}^n\,.$$

The set of all these points corresponds to the representation of $\tilde{\Lambda}$ in the tangent space at the chosen point q. Typically, if $u_q = u_o = 0$, we find :

$$\left\{\left(H(0)\,;\,\Omega(0)\,B\,\lambda\right) \mid \lambda \in \mathbb{Z}^n\right\}\,,$$

the representation of $\tilde{\Lambda}$ in the tangent space at the origin o.

Figure 3.4 shows the case of a one-dimensional modulated lattice, in the case of a modulation :

$$u \longmapsto H(u) \doteq u + A\sin(k\,u)\,,$$

with $A, k \in \mathbb{R}$. The equivalence class of any node $a\,\lambda$, where $a \in \mathbb{R}_+$, is :

$$\left(a\,\lambda + w + A\sin\left(k\,(a\,\lambda + w)\right)\,;\,-w\left[1 + k\,A\cos\left(k\,(a\,\lambda + w)\right)\right]\right)\,,$$

where $w \in \mathbb{R}$. The representation of $\tilde{\Lambda}$ in any tangent space (any "vertical" cut) yields a periodic lattice, in the sense that it is a set isomorphic to the finite free module $\mathbb{Z}$. Figure 3.5 shows how the condition that H be one-to-one is important; as soon as this condition is not satisfied, each "equivalence class" is crossing itself and others. This is due to the fact that M does not have a manifold structure any more.

3.2 Symmetry Operations in the Tangent Bundle

The equivalence relation $\sim$ on the tangent bundle of a manifold is particularly useful in the case of modulated structures, because it relates the modulated shape of such structures with the advantageous property of linearity of any tangent space. If we consider the extension of a structure in the tangent bundle, we also need to find how symmetry operations act on points of the tangent bundle, how they are represented in this space. For that, we first need to focus on several concepts related to isometries in the Euclidean manifold, such as the *symmetry element* and the *intrinsic translation*.
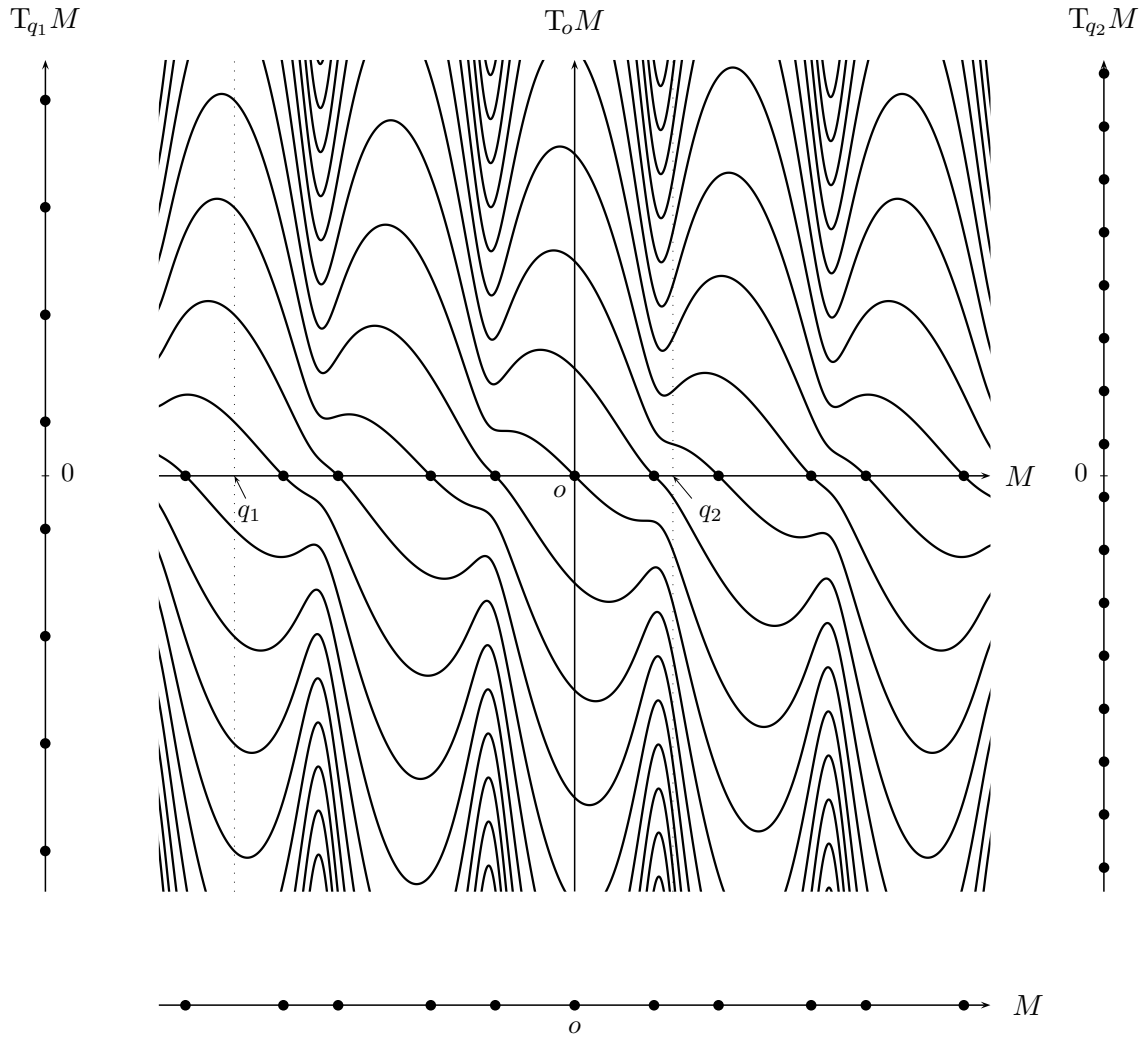
Figure 3.4:   Representation of a one-dimensional sinusoidally modulated lattice in the tangent bundle of a one-dimensional (modulated) manifold. M corresponds to $\mathbb{R}$, it is just parameterised by a map which is different from the identity. Thus, TM is just $\mathbb{R}^2$. A "vertical" cut through any point q corresponds to the representation of the lattice in the tangent space at q. Note that in such a space, the lattice is "periodic", in the sense that it is a $\mathbb{Z}$-module.
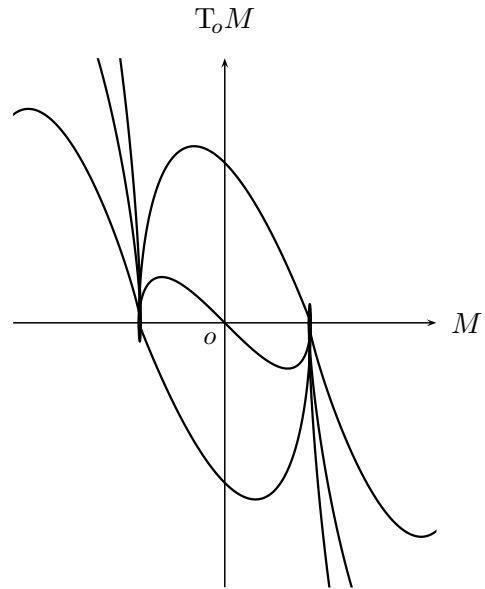
Figure 3.5: When H is not a one-to-one map from $\mathbb{R}^n$ to M (which is in fact $\mathbb{R}^n$ as well), M does not exhibit a manifold structure anymore and the definition of equivalence relation on the "tangent bundle" becomes irrelevant : two different "equivalence classes" cross at least at one point, hence they are connected.

3.2.1 Finding the Intrinsic Translation

As an introduction and motivation, we consider a concrete example. Let ϕ be an isometry in the one-dimensional Euclidean manifold (endowed with the natural coordinate system u), such that its action on any point p with coordinate u_p be

$$u_p \longmapsto -u_p + s \ ,$$

where s is a real number. Consider then the equation $u = -u + s$; its solution is $u = \frac{1}{2} s$. The point $\bar{q}$, the coordinate of which is $\frac{1}{2} s$, may be called *fixed point* because it remains unchanged through the map ϕ. As seen in the previous chapter, any isometry can also be represented by a linear map, its differential map, between two tangent space; in our case, this differential map is $\mathrm{d}\phi_q$, which carries v to v', where v and v' are the tangent vectors which represent, respectively, the point p and its image $\phi(p)$ in the tangent spaces at a point q and at its image $\phi(q)$, respectively. The expression in coordinates of $\mathrm{d}\phi_q$ is the 1×1 matrix -1. Then v' is just equal to $-v$. Such an isometry, which inverses any vector, is called *inversion operation*. Figure 3.6 shows the manifold and the tangent space representations of this operation. Their equivalence clearly appears through the $\sim$ relation. The figure also
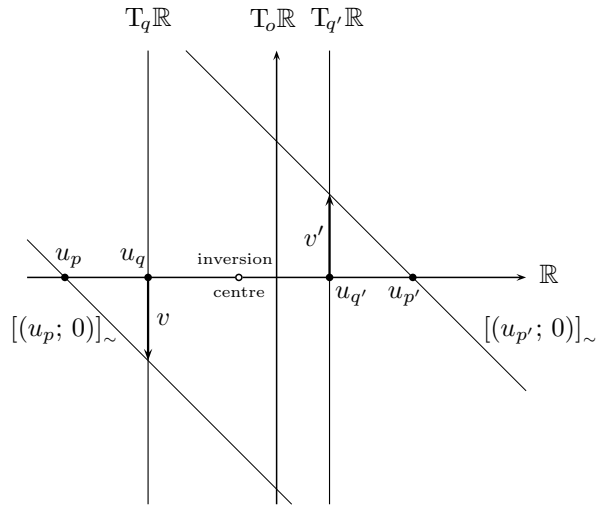
Figure 3.6: Illustration of the tangent space representation of an isometry in the one-dimensional Euclidean space. The isometry is here an inversion ϕ. The differential map $\mathrm{d}\phi_q$ carries the vector v in the tangent space at q to the vector $v' = \mathrm{d}\phi_q(v)$ in the tangent space at $q' = \phi(q)$. With the tangent bundle representation of p and p' (the equivalence classes $[(u_p; 0)]_\sim$ and $[(u_{p'}; 0)]_\sim$), we see that the tangent space representation of ϕ is completely equivalent to the usual manifold one. The fixed point $\bar{q}$ of this operation is called *inversion centre*.

shows that in the case of the representation of the point p in the tangent space at the point $\bar{q}$, the differential map $\mathrm{d}\phi_{\bar{q}}$ is an endomorphism of $\mathrm{T}_{\bar{q}}\mathbb{R}$. This fact is an additional reason why $\bar{q}$ may be called fixed point. In fact, we see that the "distance" between $\mathrm{T}_q\mathbb{R}$ and $\mathrm{T}_{\phi(q)}\mathbb{R}$ decreases when the tangent point q is closer to $\bar{q}$; it is even 0 when the chosen tangent point is $\bar{q}$. This means that if we would change the origin and would put it at $\bar{q}$, the translation part s of the operation would vanish.

With this example, we notice that the translation part depends on the choice of the origin. One might wonder if there exists a fixed point for every isometry. The answer is no, of course; a pure translation (in which case, the matrix part is the identity) has no fixed point. We conclude that the set of all Euclidean isometries can be split in two sets, one constituted of isometries containing at least one fixed point and the other constituted of isometries without a fixed point. However, for any isometry, there exists

at least one point such that the "distance" between the tangent space at this point and the tangent space at its image point, through the isometry, is minimal. As the tangent bundle of $\mathbb{R}^n$ is built as the cartesian product of $\mathbb{R}^n$ and $\mathbb{R}^n$, the distance between these two tangent spaces is nothing but the distance between the tangent point and its image. If the isometry has at least one fixed point, the distance between the two tangent spaces can be reduced to 0; the corresponding tangent point is then the fixed point. For pure translations, this distance is constant, it does not depend on the selected tangent point. Let us then see if other cases exist, where the distance between a point and its image is not constant but never vanishes. For this purpose, we consider the general form of a Euclidean isometry and look for the point p such that its distance to its image $\phi(p)$ is minimal. In order to obtain formulas applicable to crystallography, we consider a coordinate system x, with respect to which the metric tensor is not necessarily diagonal but still constant. $x = (x^1; \ldots; x^n)$ is obtained from $u = (u^1; \ldots; u^n)$ by multiplying this latter by an invertible matrix B. In the coordinate system x, a Euclidean isometry ϕ is still represented by a matrix F and translation s parts, but the matrix, although of determinant ± 1, is not orthogonal any more. In components, we have :

$$x'^i = \sum_{j=1}^{n} f^i{}_j\, x^j + s^i \ ,$$

where $f^i{}_j$ are the components $(i; j)$ of a matrix F and s^i the i-th component of s. The distance between a point q and its image $\phi(q)$ is simply the length of the straight line linking these two points. Its square is :

$$\mathrm{dist}^2\big(q;\, \phi(q)\big) = \sum_{i,j=1}^{n} \left(\sum_{k=1}^{n}(f^i{}_k - \delta^i{}_k)\, x_q{}^k + s^i \right) \left(\sum_{l=1}^{n}(f^j{}_l - \delta^j{}_l)\, x_q{}^l + s^j \right) g_{ij} \ , \qquad (3.2.1)$$

where g_{ij} are the components $(i; j)$ of the constant metric tensor in the coordinate system x. To find the minimum of this distance, we use the derivative techniques : we calculate the directional derivative of this distance, seen as a function, in the direction given by v, where v is the tangent vector at q of the straight line γ linking q to $\phi(q)$. This straight line, linearly parameterised between 0 and 1, is given by :

$$\begin{aligned} \gamma : [0\,;\, 1] &\longrightarrow \mathbb{R}^n \\ t &\longmapsto \gamma(t) = x_q + (x_{\phi(q)} - x_q)\, t \end{aligned}$$

Since a function and its square have the same extrema, we shall rather calculate the directional derivative of the square of the distance function, in order to have simpler expressions. As $\phi(q)$ completely depends on q, this distance function does not depend on the coordinates of both points q and $\phi(q)$, but only on q. We can then write $\mathrm{dist}\big(q;\, \phi(q)\big)$ as a function ϵ of the coordinates x_q, $\epsilon(x_q) \doteq \mathrm{dist}\big(q;\, \phi(q)\big)$. Thus, the directional derivative ∂_v of ϵ^2 in the direction v is :

$$\partial_v \epsilon^2 \doteq \frac{\mathrm{d}}{\mathrm{d}t}(\epsilon^2 \circ \gamma)(t)|_{t=0} = \sum_{m=1}^{n} \partial_m \epsilon^2\big(\gamma(t)\big) \left.\frac{\mathrm{d}\gamma^m(t)}{\mathrm{d}t}\right|_{t=0} = \sum_{m=1}^{n} \partial_m \epsilon^2(x_q)\, (x_{q'}{}^m - x_q{}^m) \ ,$$

where :

$$\partial_m \epsilon^2(x_q) = \frac{\partial}{\partial x^m} \epsilon^2(x_q) = 2 \sum_{i,j=1}^{n} (f^i{}_m - \delta^i{}_m) \left(\sum_{k=1}^{n} (f^j{}_k - \delta^j{}_k) x_q{}^k + s^j \right) g_{ij} \ ,$$

and :

$$(x_{q'}{}^m - x_q{}^m) = \sum_{i=1}^{n} (f^m{}_i - \delta^m{}_i) x_q{}^i + s^m \ .$$

Let us write $w^m = (x_{q'}{}^m - x_q{}^m)$ and $a^i{}_j = (f^i{}_j - \delta^i{}_j)$. Then :

$$\partial_v \epsilon^2 = 2 \sum_{i,j,m=1}^{n} a^i{}_m \, w^j \, g_{ij} \, w^m = 2 \sum_{i,j,m} g_{ij} \, a^i{}_m \, w^m \, w^j = 2 \sum_{i,j,m} g_{ij} \, w^i \, a^j{}_m \, w^m \ .$$

To obtain the last equality, we used the symmetry property of the metric tensor, $g_{ij} = g_{ji}$, for all $1 \leqslant i, j \leqslant n$. The expression obtained above can be written in a compact matrix form :

$$\partial_v \epsilon^2 = {}^{\mathrm{t}}\!\left(\nabla \epsilon^2(x_q) \right) w = {}^{\mathrm{t}}w \, G \, A \, w = {}^{\mathrm{t}}w \, G \, (F - I_n) \, w = {}^{\mathrm{t}}w \, G \, F \, w - {}^{\mathrm{t}}w \, G \, w \ ,$$

where $A = (a^i{}_j)^n_{i,j=1}$, $w = (F - I_n) \, u_q + s$ and $G = {}^{\mathrm{t}}G$ is the matrix representing the constant metric tensor in the coordinate system x. The function ϵ is extremal when

$$\partial_v \epsilon^2 = {}^{\mathrm{t}}w \, G \, F \, w - {}^{\mathrm{t}}w \, G \, w = {}^{\mathrm{t}}w \, G \, (F - I_n) \, w = 0 \ . \tag{3.2.2}$$

Note that the distance between a point and its image can never been maximal, except for the case of the pure translation, where this distance is constant. Indeed, as soon as the matrix F differs from the identity I_n, the components of $(F - I_n) \, x_q$ are not all equal to zero; thus ${}^{\mathrm{t}}[(F - I_n) \, x_q] \, G \, (F - I_n) \, x_q$, therefore the distance between q and its image $\phi(q)$, increase infinitely when the components of q grow infinitely. Then, any point q, with coordinates x_q, which satisfy equation 3.2.2 correspond to a minimum of the distance function. Notice that this equation has a trivial solution if $(F - I_n) \, w$ is perpendicular to w. As $(F - I_n) \, w = F \, w - w$ has always a component parallel to w, this can never happen, unless $w = 0$. Let us find the points q which satisfy this relation 3.2.2. Several cases may be distinguished.

1. $w = 0$ and $F = I_n$. Then :

$$w = s = 0 \ .$$

   The symmetry operation is the identity.

2. $w = 0$ and $F \neq I_n$. The symmetry operation has at least one fixed point. Indeed, we have

$$w = (F - I_n) \, x_q + s = 0 \quad \Leftrightarrow \quad F \, x_q + s = x_q \ ,$$

   what is the equation of the fixed point(s) of the symmetry operation.

3. $w \neq 0$ and $F \neq I_n$. Then ${}^t w \, G \, (F - I_n) \, w = 0$ if and only if $(F - I_n) \, w = 0$. Let $P \in \mathrm{GL}_n(\mathbb{R})$ be a matrix of basis change, such that $P \, F \, P^{-1} \doteq U$ is an orthogonal matrix, which may be written in the irreducible form [Eng86] :

$$
U = \left(
\begin{array}{ccc|ccc}
\pm 1 & & 0 & & & \\
 & \ddots & & & 0 & \\
0 & & \pm 1 & & & \\
\hline
 & & & U_1 & & 0 \\
 & 0 & & & \ddots & \\
 & & & 0 & & U_m
\end{array}
\right) \quad ,
\tag{3.2.3}
$$

where :

$$
U_i = \left(
\begin{array}{cc}
\cos \theta_i & -\sin \theta_i \\
\sin \theta_i & \cos \theta_i
\end{array}
\right) \quad , \quad 1 \leqslant i \leqslant m \; .
$$

θ_i is supposed to be different from $k \, \pi$, $k \in \mathbb{Z}$, for otherwise, U_i would be equal to $\pm I_2$ and would thus be a part of the first block of the matrix U. In our case, at least one of the values of this first block is necessarily $+1$, for otherwise, U would be invertible, which would correspond to the previous case, where $w = 0$. Suppose that the number of values $+1$ is r. Thus, we have :

$$
(F - I_n) \, w = 0 \quad \Leftrightarrow \quad P \, (F - I_n) \, P^{-1} P \, w = 0 \quad \Leftrightarrow \quad (U - I_n) \, P \, w = 0 \; ,
$$

with :

$$
U - I_n = \left(
\begin{array}{c|c}
0_r & 0_{r \times (n-r)} \\
\hline
0_{(n-r) \times r} & B
\end{array}
\right) \quad ,
$$

where B is a $(n - r) \times (n - r)$ invertible matrix. A right multiplication of the last equation above by P gives :

$$
\begin{aligned}
(F - I_n) \, w &= 0 & \Leftrightarrow \\
\Leftrightarrow \quad P \, (F - I_n) \, w &= 0 & \Leftrightarrow \\
\Leftrightarrow \quad P \, (F - I_n) \big((F - I_n) \, x_q + s \big) &= 0 & \Leftrightarrow \\
\Leftrightarrow \quad P \, (F - I_n) \, P^{-1} \big(P \, (F - I_n) \, P^{-1} P \, x_q + P \, s \big) &= 0 & \Leftrightarrow \\
\Leftrightarrow \quad (U - I_n)^2 \, P \, x_q + (U - I_n) \, P \, s &= 0 \; . &
\end{aligned}
\tag{3.2.4}
$$

Let us write the following decomposition :

$$
P \, x_q = \left(
\begin{array}{c}
(P \, x_q)_\| \\
(P \, x_q)_\perp
\end{array}
\right) \quad , \quad
P \, s = \left(
\begin{array}{c}
(P \, s)_\| \\
(P \, s)_\perp
\end{array}
\right) \quad ,
$$

where $(P \, x_q)_\|$ and $(P \, s)_\|$ contains the first r components of $P \, x_q$ and $P \, s$ respectively, and $(P \, x_q)_\perp$ and $(P \, s)_\perp$ the last $n - r$ ones. From equation 3.2.4, we obtain the following condition :

$$
B \, (P \, x_q)_\perp + (P \, s)_\perp = 0 \; .
\tag{3.2.5}
$$

Thus, we conclude that every point q such that its coordinates x_q satisfy the expression :

$$(P\,x_q)_\perp = B^{-1}\,(P\,s)_\perp \ , \tag{3.2.6}$$

is such that the distance between it and its image is minimal. Note that relation 3.2.6 consists in $n - r$ linearly independent equations which can be seen as constraints on the n coordinates of the point; this means that r of the n coordinates of the point are free, they may be chosen arbitrarily. Equation 3.2.5 shows that each of these constraints may be written as $f(x) = 0$. As P and B are invertible matrices, all the gradients of each of these functions are linearly independent. Thus,

$$\mathcal{N} = \{q \in \mathbb{R}^n \mid B\,(P\,x_q)_\perp + (P\,s)_\perp = 0\}$$

is a submanifold of $\mathbb{R}^n$ of dimension r. Notice that every point q of $\mathcal{N}$ is such that its image through the symmetry operation remains in $\mathcal{N}$. Indeed, if $x_{q'} = F\,x_q + s$, then :

$$P\,x_{q'} = P\,F\,x_q + P\,s = P\,F\,P^{-1}P\,x_q + P\,s = U\,P\,x_q + P\,s \ ,$$

and :

$$
\begin{aligned}
(P\,x_{q'})_\perp &= (U\,P\,x_q)_\perp + (P\,s)_\perp = \\
&= (B + I_{(n-r)})\,(P\,x_q)_\perp + (P\,s)_\perp = \\
&= -(P\,s)_\perp + (P\,x_q)_\perp + (P\,s)_\perp = \\
&= (P\,x_q)_\perp \ ;
\end{aligned}
$$

the coordinates of the point $q \in \mathcal{N}$ and its image are such that $(P\,x_{q'})_\perp = (P\,x_q)_\perp$, what means that both satisfy relation 3.2.5. The symmetry operation corresponding to this case has no fixed point, but it is not a pure translation as well, because we suppose that the matrix part is not equal to the identity.

4. $w \neq 0$ and $F = I_n$. The corresponding symmetry operation is a pure translation. Indeed, we have :

$$w = s \neq 0 \ .$$

The calculations and the different cases presented here are mostly treated in several textbooks, for instance in the monograph written by D. Schwarzenbach and G. Chapuis [SC06], or that of H. Burzlaff and H. Zimmermann [BZ77]. But the concepts used to obtain them are completely different. Thus, new definitions of notions commonly used in crystallography can be given.

3.2.1 Definition : A *symmetry element* of a Euclidean symmetry operation is the submanifold $\mathcal{N}$ of the Euclidean manifold composed of all points such that the distance between one of them and its image is minimal.

3.2.2 Proposition : *This submanifold $\mathcal{N}$ is invariant under the symmetry operation, its image corresponds to itself.*

3.2.3 Remark : Thanks to this proposition, our definition of symmetry element is equivalent to that commonly used, that is the set of all points which is transformed into itself through the symmetry operation.

3.2.4 Definition : The *intrinsic translation* of a Euclidean symmetry operation is the element $w = x_{q'} - x_q = (F - I_n) x_q + s$, where $q \in \mathcal{N}$ and $q' = \phi(q)$. It can be seen as the tangent vector at q of the straight line linearly parameterised between 0 and 1, linking q to $q' = \phi(q)$.

- A symmetry operation ϕ for which :

$$\min_{q \in \mathbb{R}^n} \text{dist}\big(q;\, \phi(q)\big) = 0$$

  is called a *fixed-point operation.*

- A symmetry operation ϕ for which :

$$\min_{q \in \mathbb{R}^n} \text{dist}\big(q;\, \phi(q)\big) = c > 0$$

  is called an *operation without a fixed point.*

3.2.5 Consequence : As $\phi(q) = q' \in \mathcal{N}$ when $q \in \mathcal{N}$, the intrinsic translation $w = x_{q'} - x_q$ can never be perpendicular to $\mathcal{N}$, it is always contained in $\mathcal{N}$. In other words, it is the "minimal vector of translation". Any point q which is not in $\mathcal{N}$ is such that the distance between itself and its image $\phi(q)$ is bigger than the length of w. Any point in $\mathcal{N}$ is not affected by the effect of the matrix part of the operation, but only by the translation part, whereas a point outside $\mathcal{N}$ is subject to both.

3.2.6 Remark : This shows that our definition of intrinsic translation correspond to that commonly used, that is a vector "contained" in (parallel to) the symmetry element which cannot vanish under a change of coordinates.

These definitions are particularly interesting if we consider the tangent space representation of a symmetry operation ϕ. Indeed, for any point q in the symmetry element $\mathcal{N}$ as a tangent point, the differential map $d\phi_q : T_q\mathbb{R}^n \to T_{\phi(q)}\mathbb{R}^n$ carries vectors of the tangent space at a point of $\mathcal{N}$, the point q, to the tangent space at another point of $\mathcal{N}$, the point $q' = \phi(q)$; and $x_{q'} - x_q$ corresponds to the intrinsic translation of ϕ. Thus, the intrinsic characteristics of the operation are obtained in a clear and simple way, without doing any change of coordinates! We therefore understand why the translation part s does not correspond to the intrinsic translation when the origin of the coordinate system is not in the symmetry element $\mathcal{N}$. Indeed, every point p of $\mathbb{R}^n$ may be seen as the tip of a vector v linking the origin to itself. The image of p is then simply the image of v (through the differential map of the operation) the foot point of which is at the image of the origin point. When the origin point is in $\mathcal{N}$, it is only under the effect of the intrinsic translation of the symmetry operation and it is this translation which appears in the image of the point p :

$$x_o = 0 \quad \text{and} \quad x_{o'} = w$$
$$x_p = v \quad \text{and} \quad x_{p'} = F\,v + w \;.$$

When the origin is not in $\mathcal{N}$, it is under the effect of both parts of the operation; the origin and its image are not linked by "the minimal vector of translation" w. The intrinsic translation does not appear in the image of the origin, therefore also not in the image of any point p :

$$x_o = 0 \quad \text{and} \quad x_{o'} = s$$
$$x_p = v \quad \text{and} \quad x_{p'} = F\, v + s \ .$$

As an example, let us consider the symmetry operation ϕ of the three-dimensional Euclidean space $\mathbb{R}^3$, which is given by :

$$\underbrace{\begin{pmatrix} u'^1 \\ u'^2 \\ u^3 \end{pmatrix}}_{u'} = \underbrace{\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}}_{F} \underbrace{\begin{pmatrix} u^1 \\ u^2 \\ u^3 \end{pmatrix}}_{u} + \underbrace{\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}}_{s} \quad ,$$

where $(u^1;\, u^2;\, u^3)$ is the natural coordinate system of $\mathbb{R}^n$. Some algebra shows that :

$$w = (F - I_3)\, u + s = \begin{pmatrix} -u^1 + u^2 + 1 \\ u^1 - u^2 + 1 \\ -2\, u^3 + 1 \end{pmatrix}$$

is never equal to 0. Moreover, $F \neq I_3$. We are then typically in the third case presented above. To find the symmetry element and the intrinsic translation, we use the technique described previously . If we follow the first method, we first need to find the matrix P such that $U = P\, F\, P^{-1}$ has the form of the matrix in the expression 3.2.3. This matrix is :

$$P = \frac{1}{2} \begin{pmatrix} \sqrt{2} & \sqrt{2} & 0 \\ -\sqrt{2} & \sqrt{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad .$$

Thus, we have :

$$U = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \ ,$$

and :

$$(U - I_n) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -2 & 0 \\ 0 & 0 & -2 \end{pmatrix} \ , \quad \text{with} \quad B \doteq \begin{pmatrix} -2 & 0 \\ 0 & -2 \end{pmatrix} \ .$$

Equation 3.2.5 becomes in this case :

$$\begin{pmatrix} \sqrt{2}\,(-u^1 + u^2) \\ 2\, u^3 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \ .$$

We obtain $u^1 = u^2$ and $u^3 = \frac{1}{2}$. The symmetry element of this operation is then :

$$\mathcal{N} = \{q \in \mathbb{R}^3 \mid u_q^{\ 1} = u_q^{\ 2} \ \text{and} \ u_q^{\ 3} = \tfrac{1}{2}\} \ .$$

Finally, the intrinsic translation is :

$$w = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} .$$

These results may also be found more straightforwardly, by considering equation 3.2.2. Indeed, as $F \neq I_3$, this equation is satisfied if and only if $(F - I_3)\, w = 0$. In components, this condition is :

$$\begin{pmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \begin{pmatrix} w^1 \\ w^2 \\ w^3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} .$$

Thus :

$$\left\{ \begin{array}{rcl} -w^1 + w^2 & = & 0 \\ w^1 - w^2 & = & 0 \\ -2\, w^3 & = & 0 \end{array} \right. \qquad \Leftrightarrow \qquad \left\{ \begin{array}{rcl} w^1 & = & w^2 \\ w^3 & = & 0 \end{array} \right. .$$

Note that $w = (F - I_3)\, u + s$; in components :

$$\begin{pmatrix} w^1 \\ w^2 \\ w^3 \end{pmatrix} \begin{pmatrix} -1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & -2 \end{pmatrix} \begin{pmatrix} u^1 \\ u^2 \\ u^3 \end{pmatrix} + \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} .$$

Thus :

$$\left\{ \begin{array}{rcl} w^1 & = & -u^1 + u^2 + 1 \\ w^2 & = & u^1 - u^2 + 1 \\ w^3 & = & -2\, u^3 + 1 \end{array} \right. .$$

As $w^1 = w^2$, then :

$$-u^1 + u^2 + 1 = u^1 - u^2 + 1 \qquad \Leftrightarrow \qquad u^1 = u^2 \ ,$$

what implies that $w^1 = w^2 = 1$. Thus, the intrinsic translation is :

$$w = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} .$$

Furthermore, as $w^3 = 0$, then $u^3 = \frac{1}{2}$. The symmetry element is therefore the submanifold $\mathcal{N}$, defined above, which is the set of all points the coordinates of which are such that $u^1 = u^2$ and $u^3 = \frac{1}{2}$. Notice that $\mathcal{N}$ is of dimension 1 and w is parallel to $\mathcal{N}$. Note also that the transformation of F into the irreducible matrix form U shows that the operation corresponds to a rotation of angle π. Thus, in our example, the symmetry operation ϕ is a rotation of angle π around the axis $\mathcal{N}$ combined with the (intrinsic) translation w along this axis. In crystallography, this is called a *helicoidal two-fold axis*.

3.2.2 Referring Symmetry Operations to any Origin

For the ancient Greeks, *algebra* and *geometry* were two distinct and competitive disciplines. Both had a substantial importance, as all problems of concrete life could not be systematically solved by one of these subjects alone. Since that time, in particular these last two-hundred years, more and more connections between geometry and algebra have appeared; today, geometry is essentially a part of vector spaces theory, and calculus. As a consequence, one treats geometrical problems with algebra only, and forget that one could solve them with a compass and a ruler. For instance, the Gauss-Bonnet theorem is sometimes applied to the Euclidean manifold in order to show that the sum of the angles in a triangle is equal to π, whereas this latter result can be simply obtained by drawing a parallel to a side of the triangle going through the opposite vertex.

Most of the time, isometries, especially the Euclidean ones, are also treated with algebraic tools : they are represented by a matrix and a translation part. However, crystallographers attach importance to represent crystal structures and their symmetry operations in figures and diagrams. Such geometrical (graphic) representations do not depend on the notion of coordinate system and origin, only the relative arrangement of objects between them have an importance; the symmetry element and the intrinsic translation are then the appropriate tools for describing an isometry in a diagram, as they depend on nothing else than their own characteristics. In crystallography, both, algebraic and geometrical representations of symmetry operations are important. It is then necessary to find a way to pass from one to the other. The previous section showed how to obtain the symmetry element and the intrinsic translation from the matrix and translation parts of an isometry, referred to a coordinate system. The inverse path needs to be developed. For this purpose, the tangent bundle representation of a point in the Euclidean manifold is required.

Recall that the tangent bundle representation of a point p with coordinates u_p is $(u_p - v\,;\, v)$, where $v \in \mathbb{R}^n$ is an n-dimensional parameter which corresponds to a vector of the tangent space at the point q with coordinates $u_q = u_p - v$. As a consequence of the Taylor development, the image of the point p through an isometry ϕ may be written in coordinates as :

$$F\,u_p + s = F\,(u_p - v + v) + s = F\,(u_p - v) + F\,v + s = F\,(u_p - v) + s + F\,v\;,$$

where F and s are, respectively, the matrix and translation parts of the isometry ϕ. This expression can symbolically be written as $\phi(p) = \phi(q) + \mathrm{d}\phi_q(v)$, where q is any point with coordinates $u_q = u_p - v$. Considering v and $\mathrm{d}\phi_q(v)$ as elements of tangent spaces, relation 3.2.2 should be written as :

$$\mathrm{d}\phi_q : (q\,;\, v) \longmapsto \big(\phi(q)\,;\, \mathrm{d}\phi_q(v)\big)\;.$$

As v is a free parameter, $\mathrm{d}\phi_q$ is a map not only between one but between any tangent space and its image. We shall write it $\mathrm{d}\phi$ instead of $\mathrm{d}\phi_q$. It is in fact a function between elements of the tangent bundle.

3.2.7 Lemma : *Let $\mathbb{R}^n$ be the Euclidean manifold, endowed with the natural coordinate system u, ϕ a Euclidean isometry and $\mathrm{d}\phi$ its differential map at any point. Then,*

dϕ carries the tangent bundle representation (equivalence class) of any point p to the tangent bundle representation (equivalence class) of its image $\phi(p)$.

Indeed :

$$\mathrm{d}\phi : \begin{pmatrix} u_p - v \\ v \end{pmatrix} \longmapsto \begin{pmatrix} F(u_p - v) + s \\ F\,v \end{pmatrix} \quad , \tag{3.2.7}$$

where F and s are, respectively, the matrix and translation parts of ϕ; note that F is also the matrix representing dϕ at any point. Now, $F(u_p - v) + s = (F\,u_p + s) - F\,v$; then :

$$\bigl(F(u_p - v) + s \,;\; F\,v\bigr)$$

belongs to the equivalence class of $(F\,u_p + s\,;\; 0)$. ■

3.2.8 Definition : dϕ, as represented in expression 3.2.7, is called the *tangent bundle representation* of the isometry ϕ.

3.2.9 Remark : dϕ can be written in the following matrix notation :

$$\begin{pmatrix} u_p - v \\ v \end{pmatrix} \longmapsto \begin{pmatrix} F & 0_n \\ 0_n & F \end{pmatrix} \begin{pmatrix} u_p - v \\ v \end{pmatrix} + \begin{pmatrix} s \\ 0 \end{pmatrix} . \tag{3.2.8}$$

In order to motivate and illustrate the considerations above, we take the example of the isometry ϕ in the two-dimensional Euclidean manifold $\mathbb{R}^2$, endowed with the natural coordinate system $u = (u^1; u^2)$, which consists in a reflexion through the mirror line $(u^1; u^1)$ cutting u^1 at a, followed by the translation $(b; b)$. In crystallography, such an isometry is called glide plane. As the translation is parallel to the mirror line, it corresponds to the intrinsic translation. The aim is to find the matrix and translation part of this glide plane in the coordinate system $(u^1; u^2)$. The matrix part F is easily obtained by using some basic linear algebra :

$$F = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad .$$

To obtain the translation part, we could perform a change of coordinates in order to have the new origin on the symmetry element, find the expression of the isometry in this new coordinates system, and return to the previous one. Such a method is perfectly correct, but long and cumbersome. By using the tangent bundle representations of points and symmetry operations, we can reach the same result without considering any change of coordinates. Indeed, let o be the origin of the coordinate system, the coordinates of which are $u_o = (0; 0)$. Its tangent bundle representation is $(-v^1, -v^2; v^1, v^2)$. Through dϕ, it becomes :

$$\begin{pmatrix} -v^1 \\ -v^2 \\ v^1 \\ v^2 \end{pmatrix} \longmapsto \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -v^1 \\ -v^2 \\ v^1 \\ v^2 \end{pmatrix} + \begin{pmatrix} s^1 \\ s^2 \\ 0 \\ 0 \end{pmatrix} .$$

Let $-v = (a\,; 0)$. The point q, such that $u_q = -v = (a\,; 0)$, lies on the glide plane; its image is then obtained by adding the intrinsic translation to its coordinates : $u_{q'} = (a\,; 0) + (b\,; b) = (a + b\,; b)$. Thus, we have the equation :

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ 0 \end{pmatrix} + \begin{pmatrix} s^1 \\ s^2 \end{pmatrix} = \begin{pmatrix} a + b \\ b \end{pmatrix} ,$$

from which we derive :

$$\begin{pmatrix} s^1 \\ s^2 \end{pmatrix} = \begin{pmatrix} a + b \\ -a + b \end{pmatrix} ,$$

the translation part of the isometry in the coordinate system under consideration.

This example shows the importance of the points which belongs to the symmetry element of a Euclidean isometry. Thanks to them, it is possible to obtain the image of any point without knowing the translation part s. Moreover, a relation between the translation part s and the intrinsic translation w can be easily derived. Indeed, for any point q with coordinates u_q, lying on the symmetry element of an isometry ϕ, its image through this latter can be written as $F\,u_q + s$, as well as $u_q + w$, where F, s and w are respectively the matrix part, the translation part, and the intrinsic translation of ϕ. The first expression is the usual one for the image of any point through the isometry, while the second is a consequence of the fact that q belongs to the symmetry element. Thus, if we equalise these two forms, we obtain :

$$F\,u_q + s = u_q + w \quad \Leftrightarrow$$

$$\Leftrightarrow \quad s = (I_n - F)\,u_q + w , \tag{3.2.9}$$

The coordinates of the image of any point p, with coordinates u_p, are then :

$$F\,u_p + (I_n - F)\,u_q + w .$$

Indeed :

$$
\begin{aligned}
F\,u_p + s &= F\,(u_q + v) + s = F\,u_q + s + F\,v = \\
&= u_q + w + F\,v = u_q + w + F\,(u_p - u_q) = \\
&= F\,u_p + (I_n - F)\,u_q + w .
\end{aligned}
$$

The tangent bundle representation of points and Euclidean isometries are very useful tools because they offer a framework which is independent of the choice of the origin. Even without performing any change of origin, we can obtain the representation of an isometry as if the origin would be at any other place, for instance on the symmetry element. We have already seen that any isometry can be seen as a map in the Euclidean manifold, as well as a linear map between two tangent spaces. Thanks to the tangent bundle formalism, we observe that it can finally also be a map from a tangent space into itself. Indeed, let p be a point with coordinates u_p and ϕ an isometry. The tangent

Figure 3.7: In coordinates, the inversion operation ϕ, with inversion centre at $(a; 0)$, is written as $u' = -u + s$, where s ($= 2a \in \mathbb{R}_+$) is the translation part. This latter corresponds to the distance between the tangent space $T_o\mathbb{R}$ at the origin o and the tangent space $T_{\phi(o)}\mathbb{R}$ at the image of the origin $\phi(o)$. In the tangent space representation of this operation, the vector $v \in T_o\mathbb{R}$ is carried to the vector $v' \in T_{\phi(o)}\mathbb{R}$. Thanks to the equivalence relation $\sim$ on the tangent bundle, $v' \in T_{\phi(o)}\mathbb{R}$ is equivalent to the vector $v'' \in T_o\mathbb{R}$. The length of this vector v'' is nothing else than the sum of the length of v' (which is equal to the length of v) and the translation part s. The value of v'' then corresponds to that between u_o and $u_{p'}$. Thus, we can write $v'' = -v' + s$, what is the same formula as for the coordinate u in the manifold.
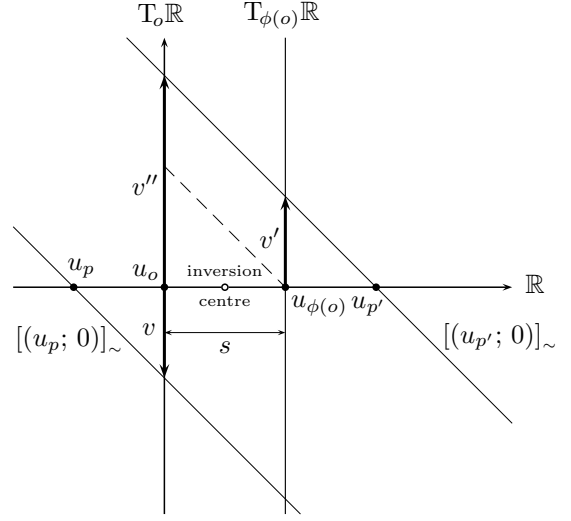
bundle representation of p is given by $(u_p - v \, ; v)$, where $v \in \mathbb{R}^n$, and is transformed, through $\mathrm{d}\phi$, according to :

$$T_q\mathbb{R}^n \qquad \longrightarrow \qquad T_{\phi(q)}\mathbb{R}^n$$

$$\begin{pmatrix} u_q \\ v \end{pmatrix} \quad \longmapsto \quad \begin{pmatrix} F\,u_q + s \\ F\,v \end{pmatrix} \, ,$$

where $u_q = u_p - v$, and F and s are respectively the matrix and translation parts of ϕ. With the $\sim$ equivalence relation, we obtain the equivalent image point in the tangent space at q :

$$\begin{pmatrix} F\,u_q + s \\ F\,v \end{pmatrix} \sim \begin{pmatrix} F\,u_q + s - \big((F - I_n)\,u_q + s\big) \\ F\,v + \big((F - I_n)\,u_q + s\big) \end{pmatrix} =$$

$$= \begin{pmatrix} u_q \\ F\,v + \big((F - I_n)\,u_q + s\big) \end{pmatrix} = \begin{pmatrix} u_q \\ F\,v + s' \end{pmatrix} \, ,$$

where $s' = (F - I_n)\,u_q + s$. Thus, we effectively obtain a map which transforms a vector $v \in T_q\mathbb{R}^n$ into the element $F\,v + s' \in T_q\mathbb{R}^n$. In particular, in the case of the tangent space at the real origin o of the coordinate system, we obtain :

$$T_o\mathbb{R}^n \qquad \longrightarrow \qquad T_{\phi(o)}\mathbb{R}^n$$

$$\begin{pmatrix} 0 \\ v \end{pmatrix} \quad \longmapsto \quad \begin{pmatrix} s \\ F\,v \end{pmatrix} \, ,$$

and :

$$\begin{pmatrix} s \\ F\,v \end{pmatrix} \sim \begin{pmatrix} 0 \\ F\,v + s \end{pmatrix}\,.$$

The image of the vector v is exactly the same as that of any point in the Euclidean manifold. We can then conclude that the Euclidean manifold and its tangent space at the origin are really the same spaces! However, a conceptual difference remains : the Euclidean space is a manifold and its tangent space at the origin is a vector space. Euclidean isometries are affine maps in the Euclidean manifold and linear maps between tangent spaces. The translation part s appearing in the expression above is due to the $\sim$, which offers the possibility to go back to the original tangent space. Figure 3.7 illustrate this point for a one-dimensional Euclidean manifold.

3.2.3 Generalisation to the Modulated Case

Recall that for the geometrical description of modulated structures, we consider a manifold M, parameterised by the one-to-one function $H : \mathbb{R}^n \to M$, such that $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$. Any symmetry operation of a modulated structure $\tilde{\mathcal{S}}$ can be written as $\tilde{\phi} \doteq H \circ \phi \circ H^{-1}$, where ϕ is a Euclidean isometry which is a symmetry operation of the corresponding average structure $\mathcal{S}$ in the Euclidean manifold. Thus, there is no need to develop a formalism for finding the symmetry element and the intrinsic translation of an operation in this case; they are simply obtained by applying respectively the parameterisation H to the symmetry element and the intrinsic translation of the corresponding Euclidean isometry ϕ. Indeed, since a symmetry operation of a modulated structure is given by $\tilde{\phi} = H \circ \phi \circ H^{-1}$, where ϕ is a Euclidean isometry with symmetry element $\mathcal{N}$ and intrinsic translation w, then $H(\mathcal{N})$ is the symmetry

Figure 3.8: Illustration of the tangent space representation of the map $\tilde{\phi} = H \circ \phi \circ H^{-1}$ in the one-dimensional manifold M parameterised by the map H, in the case where ϕ is an inversion operation. The differential map $d\tilde{\phi}_q$ carries the vector $\tilde{v}$ in the tangent space at q to the vector $\tilde{v}' = d\tilde{\phi}_{q'}(\tilde{v})$ in the tangent space at q', the image point of q through $\tilde{\phi}$. When q is on the symmetry element, $d\tilde{\phi}$ is an endomorphism of $T_q M$, what implies that the image of the vector $\tilde{v}''$ is simply $-\tilde{v}''$. With the tangent bundle representation of p and p', we notice that the tangent space representation of $\tilde{\phi}$ is completely equivalent to the usual manifold one.

element of $\tilde{\phi}$ and $H(u_q + w) - H(u_q)$, where $q \in \mathcal{N}$, its intrinsic translation. Thus, symmetry elements such as axes or mirrors are not straight lines or planes any more, and the intrinsic translation is not constant, it depends of the point $q \in \mathcal{N}$. Note that this
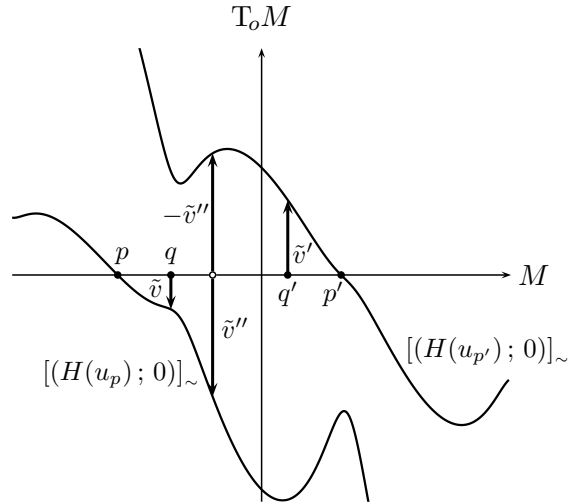
holds not only for symmetry operations of a structure $\tilde{\mathcal{S}}$ but also for any transformation from M to M which can be written as $H \circ \phi \circ H^{-1}$, where ϕ is a Euclidean isometry.

Let ϕ be a Euclidean symmetry operation of a structure $\mathcal{S}$ in the Euclidean space and $\tilde{\phi} = H \circ \phi \circ H^{-1} : M \to M$ be a symmetry operation of the corresponding modulated structure $\tilde{\mathcal{S}} = H(\mathcal{S})$ in the manifold M. Let also $q \in M$ be a point with coordinates $H(u_q)$. Recall that the differential map $\mathrm{d}\tilde{\phi} = \mathrm{d}H \circ \mathrm{d}\phi \circ \mathrm{d}H^{-1}$ carries any vector $\tilde{v}$ in the tangent space at q to the vector $\mathrm{d}\tilde{\phi}(\tilde{v})$ in the tangent space at the point q' with coordinates $H(u_{q'}) = H(F\,u_q + s)$, where F and s are respectively the matrix and translation parts of the isometry ϕ (see figure 3.8). Suppose that the point $\big(H(u_q)\,;\,\tilde{v}\big)$ belongs to the equivalence class of $\big(H(u_p)\,;\,0\big)$, where p is a point with coordinates $H(u_p)$. This means that $\tilde{v} = \Omega(u_q)\,(u_p - u_q)$, where Ω is the matrix representation of the differential map $\mathrm{d}H$. Considering $v \doteq u_p - u_q$ as a free n-dimensional parameter, $\mathrm{d}\tilde{\phi}_q$ becomes a function on the tangent bundle; as in the Euclidean case, we shall write $\mathrm{d}\tilde{\phi}$ instead of $\mathrm{d}\tilde{\phi}_q$. Figure 3.8 illustrate the situation in the case where ϕ is an inversion operation.

3.2.10 Lemma : *Let M be a manifold parameterised by the one-to-one map $H :$ $\mathbb{R}^n \to M$, such that $M \subset \mathbb{R}^n$ and $\mathbb{R}^n \subset M$. Let $\tilde{\phi} : M \to M$ be a map such that $\tilde{\phi} = H \circ \phi \circ H^{-1}$, where ϕ is a Euclidean isometry. Then, the differential map $\mathrm{d}\tilde{\phi} = \mathrm{d}H \circ \mathrm{d}\phi \circ \mathrm{d}H^{-1}$ of $\tilde{\phi}$ carries the tangent bundle representation (equivalence class) of any point of M to the tangent bundle representation (equivalence class) of its image through $\tilde{\phi}$.*

Indeed :

$$
\mathrm{d}\tilde{\phi} : \begin{pmatrix} H(u_p - v) \\ \Omega(u_p - v)\,v \end{pmatrix} \longmapsto \begin{pmatrix} H\big(F\,(u_p - v) + s\big) \\ \Omega\big(F\,(u_p - v) + s\big)\,F\,v \end{pmatrix} \quad , \tag{3.2.10}
$$

where F and s are respectively the matrix and translation parts of ϕ, and Ω is the matrix representing $\mathrm{d}H$. Then, writing $F\,(u_p - v) + s = (F\,u_p + s) - F\,v$, we have :

$$
\begin{pmatrix} H\big(F\,(u_p - v) + s\big) \\ \Omega\big(F\,(u_p - v) + s\big)\,F\,v \end{pmatrix} \sim \begin{pmatrix} H\big(F\,(u_p - v) + s + F\,v\big) \\ \Omega\big(F\,(u_p - v) + s + F\,v\big)\,(F\,v - F\,v) \end{pmatrix} \quad ;
$$

The first component is equal to $H(F\,u_p + s)$ and the second is 0. Thus :

$$
\big(H(F\,u_p + s)\,;\ \Omega\big(F\,(u_p - v) + s\big)\,F\,v\big)
$$

belongs to the equivalence class of $\big(H(F\,u_p + s)\,;\,0\big)$.   ∎

3.2.11 Definition : $\mathrm{d}\tilde{\phi}$, as represented in expression 3.2.10, is called the *tangent bundle representation* of the map $\tilde{\phi}$.

3.2.12 Remark : Contrary to the Euclidean case, $\mathrm{d}\tilde{\phi}$ cannot be written in matrix notation. This is due to the fact that H is (in general) not linear.

3.3 Tangent Bundle Representation of Space Groups

The choice of the origin in space groups representations is a recurring problem in crystallography. For any symmetry operation, it is advantageous to have the origin on its symmetry element. But the problem is that the different symmetry elements of the operations composing a space group do not, in general, intersect all in one point. Therefore, no privileged point exists and therefore compromises must be accepted. With the formalism developed in the previous section, this problem disappears, as any point can be chosen as an origin, without changing the real origin of the coordinate system. Each symmetry operation can then be described relatively to its own "origin" point, which can be selected among the points of its symmetry element.

3.3.1 Conventions in the International Tables

In the International Tables for Crystallography, all the plane and space groups are represented by diagrams showing the shape of the typical unit cell associated with the group, the symmetry elements and the intrinsic translations associated with the symmetry operations composing the group [ITa02, ITb02]. For space groups describing the symmetry of three-dimensional crystal structures, these figures are two-dimensional projections of three-dimensional parallelepipeds containing the symmetry elements and the intrinsic translations. Thus, for most of them, the three projections along the three axes are represented.

For each plane or space group, an origin is selected and a compact matrix representation for every symmetry operation is given. Among all existing three-dimensional symmetry operations, an order of importance is established, in order to fix a rule for the choice of the site of the origin point. It is a pure convention based on conveniences of calculations. The priority is given to the *inversion operation*, characterised by a matrix part $-I_3$ and an intrinsic translation 0; if a space (or plane) group contains an inversion operation, the origin is selected on its symmetry element, which is called the *inversion centre*. In this way, the matrix and translation parts of all symmetry operations of space groups containing an inversion operation can be deduced in a more straightforward way.

The two-dimensional diagrams representing the plane and space groups have the advantage that they do not depend on any origin point. However, for specific calculations, such representations are less useful, an algebraic expression for symmetry operation, which unfortunately depends on the choice of an origin point, is necessary.

The tangent bundle representation of Euclidean isometries offers the advantages of both representations : it is an algebraic expression which does not depend any more of the choice of the origin. Thanks to the combination of the manifold and tangent space representation of an isometry, any symmetry operation can be referred to any origin point. This implies that each operation can be expressed with respect to its own origin point which is, for evident reasons, chosen on the symmetry element. Thus, all the symmetry operations of a space group have a friendly algebraic representation, in which only the intrinsic characteristics appear. Furthermore, the relative positions of all symmetry elements can easily be obtained.

3.3.2   The Example of the Space Group $\mathrm{P2_1/c}$

The capital letter P, which is an abbreviation for *primitive*, indicates that the unit cell has the smallest possible volume and is therefore not centred. The symbol $2_1/c$, composed of two parts which correspond, in addition to the lattice translations, to the generators of the space group, *i.e.* the symmetry operations which generate all the others in the group. The crystal system, to which the space group belongs, can be directly deduced from the number and the kind of generators; in this case, the crystal system is *monoclinic*, which means that the three vectors (in a tangent space) characterising the unit cell can have any length, and two of the three angles between them must be equal to $\frac{\pi}{2}$. These three vectors are usually noted a, b and c. According to the conventions of the International Tables for Crystallography [ITb02], the angles $\frac{\pi}{2}$ are between c and b and between a and b. The symmetry operation corresponding to the symbol 2_1 is a rotation around the vector b, followed by a translation of one-half of the length of b, along the direction of this vector; the corresponding symmetry element is an axis (a one-dimensional subspace), the rotation axis, parallel to b. The operation corresponding to the symbol c is a reflection, the symmetry element of which, the mirror plane, is normal to b, followed by a translation of one-half of the vector c. Let x be a coordinate system adapted to the geometry of the unit cell, *i.e.* a coordinate system of which the associated canonical basis, in any tangent space, is the set of vectors $\{a; b; c\}$. The matrix and intrinsic translation parts of the two symmetry operations 2_1 and c are :

$$2_1 \; : \; \left\{ F_1 = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \; ; \; w_1 = \begin{pmatrix} 0 \\ \frac{1}{2} \\ 0 \end{pmatrix} \right\}$$

and

$$c \; : \; \left\{ F_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \; ; \; w_2 = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix} \right\} \; .$$

Let o be the origin point of the coordinate system ($x_o = 0$), and q the point with coordinates x_q which lies at the intersection of the rotation axis and the mirror plane. The tangent bundle representation of o is $(-v; v)$, where $v \in \mathbb{R}^n$ is a parameter. This class also contains the point $(x_q; -x_q)$. Its image through the tangent bundle representation of the 2_1 operation is :

$$\begin{pmatrix} F_1 & 0_3 \\ 0_3 & F_1 \end{pmatrix} \begin{pmatrix} x_q \\ -x_q \end{pmatrix} + \begin{pmatrix} s_1 \\ 0 \end{pmatrix} = \begin{pmatrix} F_1\, x_q + s_1 \\ -F_1\, x_q \end{pmatrix} \, ,$$

where s_1 is the translation part of 2_1 in the coordinate system x (with the chosen origin o). As q is on the symmetry element of 2_1, the coordinates of its image are simply $x_q + w_1$. Thus :

$$\begin{pmatrix} F_1\, x_q + s_1 \\ -F_1\, x_q \end{pmatrix} = \begin{pmatrix} x_q + w_1 \\ -F_1\, x_q \end{pmatrix} \, ,$$

which is equivalent to :

$$\begin{pmatrix} x_q + w_1 - w_1 \\ -F_1\, x_q + w_1 \end{pmatrix} = \begin{pmatrix} x_q \\ -F_1\, x_q + w_1 \end{pmatrix} \; ;$$

we write the equivalence as follows :

$$\begin{pmatrix} x_q + w_1 \\ -F_1\, x_q \end{pmatrix} \sim \begin{pmatrix} x_q \\ -F_1\, x_q + w_1 \end{pmatrix} .$$

Through the tangent bundle representation of the c glide plane, the image of this latter point is :

$$\begin{pmatrix} F_2 & 0_3 \\ 0_3 & F_2 \end{pmatrix} \begin{pmatrix} x_q \\ -F_1\, x_q + w_1 \end{pmatrix} + \begin{pmatrix} s_2 \\ 0 \end{pmatrix} =$$

$$= \begin{pmatrix} F_2\, x_q + s_2 \\ -F_2\, F_1\, x_q + F_2\, w_1 \end{pmatrix} ,$$

where s_2 is the translation part of the c operation in the considered coordinate system x. As q is in the mirror plane, the coordinates of its image are $x_q + w_2$. Thus :

$$\begin{pmatrix} F_2\, x_q + s_2 \\ -F_2\, F_1\, x_q + F_2\, w_1 \end{pmatrix} = \begin{pmatrix} x_q + w_2 \\ -F_2\, F_1\, x_q + F_2\, w_1 \end{pmatrix}$$

and

$$\begin{pmatrix} x_q + w_2 \\ -F_2\, F_1\, x_q + F_2\, w_1 \end{pmatrix} \sim \begin{pmatrix} x_q + w_2 + F_2\, w_1 \\ -F_2\, F_1\, x_q \end{pmatrix} .$$

If we have a look at the vector part of the equivalence class, we see that $-x_q$ is transfered to $-F_2\, F_1\, x_q = x_q$. This shows that the composition of the two operations corresponds to an inversion operation, which is represented by the symbol $\bar{1}$. Its symmetry element, the inversion centre, is located half way between q, with coordinates u_q, and the point of coordinates $x_q + w_2 + F_2\, w_1$. Referring to the convention for symmetry elements, this symmetry element should be at the origin of the coordinate system, which implies that $x_q + w_2 + F_2\, w_1$ must be equal to $-x_q$. The coordinates of q must then be :

$$x_q = -\frac{1}{2}\,(F_2\, w_1 + w_2) = \begin{pmatrix} 0 \\ \frac{1}{4} \\ -\frac{1}{4} \end{pmatrix} ;$$

They indicate the precise position of the axis and the mirror plane. This result is in agreement with the space group information given in the International Tables. Note that the coordinates of the point q were obtained without calculating the translation parts s_1 and s_2 but just using the intrinsic characteristics of each symmetry operation. s_1 and s_2 can be found by using relation 3.2.9 :

$$s_1 = -(F_1 - I_3)\, x_q + w_1 = \begin{pmatrix} 0 \\ \frac{1}{2} \\ -\frac{1}{2} \end{pmatrix} ,$$

$$s_2 = -(F_2 - I_3)\, x_q + w_2 = \begin{pmatrix} 0 \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} ;$$

the translation part s_3 of the inversion operation is of course zero. With all these considerations, we are in a position to write the tangent bundle representation of the symmetry operations 2_1, c and $\bar{1}$. For any point p, with coordinates u_p, we have :

$$2_1 \; : \; \begin{pmatrix} u_p - v \\ v \end{pmatrix} \longmapsto \begin{pmatrix} F_1 & 0_3 \\ 0_3 & F_1 \end{pmatrix} \begin{pmatrix} u_p - v \\ v \end{pmatrix} + \begin{pmatrix} s_1 \\ 0 \end{pmatrix} = \begin{pmatrix} F_1 \, (u_p - v) + s_1 \\ F_1 \, v \end{pmatrix} \; ,$$

$$c \; : \; \begin{pmatrix} u_p - v \\ v \end{pmatrix} \longmapsto \begin{pmatrix} F_2 & 0_3 \\ 0_3 & F_2 \end{pmatrix} \begin{pmatrix} u_p - v \\ v \end{pmatrix} + \begin{pmatrix} s_2 \\ 0 \end{pmatrix} = \begin{pmatrix} F_2 \, (u_p - v) + s_2 \\ F_2 \, v \end{pmatrix} \; ,$$

$$\bar{1} \; : \; \begin{pmatrix} u_p - v \\ v \end{pmatrix} \longmapsto \begin{pmatrix} -I_3 & 0_3 \\ 0_3 & -I_3 \end{pmatrix} \begin{pmatrix} u_p - v \\ v \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -(u_p - v) \\ -v \end{pmatrix} \; .$$

In these representations, any point p is seen as the tip of a tangent vector at the "origin" point q with coordinates $u_q = u_p - v$. As $v \in \mathbb{R}^3$ is a free parameter, the point q can be any point of the Euclidean manifold $\mathbb{R}^n$. Whatever this point is, the final image of the point p in the manifold is always the same. Thus, for each operation, a different origin point may be selected; this origin is preferably a point of the symmetry element of the operation, in order that its image have a very simple expression in which the characteristic parts of the operation appear only. In the present example, if we take q, with coordinates $u_q = (0; \frac{1}{4}; -\frac{1}{4})$, as an origin for the 2_1 and c operations, and the point o, with coordinates $u_o = (0; 0; 0)$ as an origin for the $\bar{1}$ operation, we obtain :

$$2_1 \; : \; \begin{pmatrix} u_q \\ u_p - u_q \end{pmatrix} \longmapsto \begin{pmatrix} u_q + w_1 \\ F_1 \, (u_p - u_q) \end{pmatrix} \; ,$$

$$c \; : \; \begin{pmatrix} u_q \\ u_p - u_q \end{pmatrix} \longmapsto \begin{pmatrix} u_q + w_2 \\ F_2 \, (u_p - u_q) \end{pmatrix} \; ,$$

$$\bar{1} \; : \; \begin{pmatrix} 0 \\ u_p \end{pmatrix} \longmapsto \begin{pmatrix} 0 \\ -u_p \end{pmatrix} \; .$$

Not one but two different origins are chosen for the tangent bundle representation of the three symmetry operations. This does not cause any problem at all, the final result in the manifold is always the same, while each symmetry operation has a representation where only its intrinsic characteristics appear.

Finally note that more than one inversion centre, one 2_1 screw-axis and one c glide-plane appear in a unit cell. These additional symmetry elements correspond to additional similar symmetry operations which are obtained by combining the three operations treated above with lattice translations. The positions of these elements may be found by using the technique of minimising the distance between a point and its image.

Chapter 4

Lattices and Point Groups

The set of all Euclidean symmetry operations is infinite and not countable; indeed, for the translation part s alone there is already a non countable infinity of possible values. Among all these isometries, most of them do not correspond to a symmetry operation of a lattice or a crystal structure. From chapter 2, we already know that the translation part of any symmetry operation must be an element of a $\mathbb{Z}$-module. But the matrix part has not been discussed yet. The goal of this chapter is to study the criteria that an isometry must satisfy in order to be a symmetry operation of a lattice of translations in the Euclidean space. Again, the modulated case does not need to be treated, since symmetry operations of modulated structures are obtained by considering the Euclidean symmetry operations of the corresponding average structure.

4.1 The Orthogonal Group as a Lie Group

In chapter 2, we have seen that the subgroup of translations in the Euclidean isometry group is a Lie group, that is a manifold which has the structure of a group. Thus, any two translations can be linked by a smooth curve, called one-parameter subgroup. The question is to know if the whole Euclidean isometry group can be endowed with a manifold structure. In order to answer this question, we need to study in detail the matrix part of a Euclidean isometry.

4.1.1 Decomposition of an Orthogonal Matrix

In any coordinate system of the Euclidean manifold, in which the metric tensor is constant, a Euclidean isometry is represented by a matrix and a translation. Such a coordinate system may be chosen arbitrarily, as the corresponding matrix and translation parts always describe the same isometry. For our purpose, we shall select a natural coordinate system, in which the metric tensor is represented by the identity matrix. Thus, the matrix part of any isometry is orthogonal, and the study of the matrix parts essentially consists in the study of the set of orthogonal matrices.

The determinant of such matrices is either $+1$ or -1. Thus, we immediately conclude that there are orthogonal matrices which cannot be linked by a smooth curve. Indeed,

as there exists no matrix the determinant of which is at the same time $+1$ and -1, there is no smooth curve in the set of orthogonal matrices linking a matrix of determinant $+1$ to another of determinant -1. Let us discuss this point more precisely by proving the following fundamental result.

4.1.1 Theorem : *Let* $O_n(\mathbb{R})$ *be the set of all real orthogonal* $n \times n$ *matrices. Then, any matrix* $F \in O_n(\mathbb{R})$ *can be written as a product of* $\frac{n}{2}(n-1)$ *orthogonal matrices :*

$$F = F(\theta^{12}; \ldots; \theta^{n-1,n}) = E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\theta^{ab}) \ ,$$

where $R_{ab}(\theta^{ab})$ *is an orthogonal matrix of the form :*

$$R_{ab}(\theta^{ab}) = \begin{pmatrix} I_r & 0_{r\times 1} & 0_{r\times s} & 0_{r\times 1} & 0_{r\times t} \\ 0_{1\times r} & \cos\theta^{ab} & 0_{1\times s} & -\sin\theta^{ab} & 0_{1\times t} \\ 0_{s\times r} & 0_{s\times 1} & I_s & 0_{s\times 1} & 0_{s\times t} \\ 0_{1\times r} & \sin\theta^{ab} & 0_{1\times s} & \cos\theta^{ab} & 0_{1\times t} \\ 0_{t\times r} & 0_{t\times 1} & 0_{t\times s} & 0_{t\times 1} & I_t \end{pmatrix} \ , \qquad (4.1.1)$$

with $r = a - 1$, $s = b - a - 1$ *and* $t = n - b$, *and*

$$E \in \{\mathrm{diag}(1; 1; 1; \ldots; 1)\,;\ \mathrm{diag}(-1; 1; 1; \ldots; 1)\} \ .$$

Proof : Let $F \in O_n(\mathbb{R})$ be an orthogonal matrix, the explicit form of which is :

$$F = \begin{pmatrix} f^1_{\ 1} & f^1_{\ 2} & \cdots & f^1_{\ n-1} & f^1_{\ n} \\ f^2_{\ 1} & f^2_{\ 2} & \cdots & f^2_{\ n-1} & f^2_{\ n} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ f^{n-1}_{\ 1} & f^{n-1}_{\ 2} & \cdots & f^{n-1}_{\ n-1} & f^{n-1}_{\ n} \\ f^n_{\ 1} & f^n_{\ 2} & \cdots & f^n_{\ n-1} & f^n_{\ n} \end{pmatrix} \ .$$

Let $R_1 \in O_n(\mathbb{R})$ be the matrix given by :

$$R_1 = \begin{pmatrix} I_{n-2} & 0_{(n-2)\times 1} & 0_{(n-2)\times 1} \\ 0_{1\times(n-2)} & \cos\theta_1 & -\sin\theta_1 \\ 0_{1\times(n-2)} & \sin\theta_1 & \cos\theta_1 \end{pmatrix} \ .$$

We can write $F = F_1 R_1$, where $F_1 = F\, {}^tR_1$. Explicitly :

$$F_1 = \begin{pmatrix} f^1_{\ 1} & \cdots & f^1_{\ n-1}\cos\theta_1 - f^1_{\ n}\sin\theta_1 & f^1_{\ n-1}\sin\theta_1 + f^1_{\ n}\cos\theta_1 \\ \vdots & \ddots & \vdots & \vdots \\ f^{n-1}_{\ 1} & \cdots & f^{n-1}_{\ n-1}\cos\theta_1 - f^{n-1}_{\ n}\sin\theta_1 & f^{n-1}_{\ n-1}\sin\theta_1 + f^{n-1}_{\ n}\cos\theta_1 \\ f^n_{\ 1} & \cdots & f^n_{\ n-1}\cos\theta_1 - f^n_{\ n}\sin\theta_1 & f^n_{\ n-1}\sin\theta_1 + f^n_{\ n}\cos\theta_1 \end{pmatrix} \ .$$

In the case where $f^n_{\ n-1}\cos\theta_1 - f^n_{\ n}\sin\theta_1 = 0$, that is when $\mathrm{tg}\,\theta_1 = \frac{f^n_{\ n-1}}{f^n_{\ n}}$, we obtain :

$$F_1 = \begin{pmatrix} f^1_{\ 1} & \cdots & f^1_{\ n-1}\cos\theta_1 - f^1_{\ n}\sin\theta_1 & f^1_{\ n-1}\sin\theta_1 + f^1_{\ n}\cos\theta_1 \\ \vdots & \ddots & \vdots & \vdots \\ f^{n-1}_{\ 1} & \cdots & f^{n-1}_{\ n-1}\cos\theta_1 - f^{n-1}_{\ n}\sin\theta_1 & f^{n-1}_{\ n-1}\sin\theta_1 + f^{n-1}_{\ n}\cos\theta_1 \\ f^n_{\ 1} & \cdots & 0 & f^n_{\ n-1}\sin\theta_1 + f^n_{\ n}\cos\theta_1 \end{pmatrix} \ .$$

Let us write $F_1 \doteq (\bar{f}^i{}_j)^n_{i,j=1}$ and consider the matrix F_2 such that $F_1 = F_2 R_2$, where $R_2 \in O_n(\mathbb{R})$ is given by :

$$R_2 = \begin{pmatrix} I_{n-3} & 0_{(n-3)\times 1} & 0_{(n-3)\times 1} & 0_{(n-3)\times 1} \\ 0_{1\times(n-3)} & \cos\theta_2 & 0 & -\sin\theta_2 \\ 0_{1\times(n-3)} & 0 & 1 & 0 \\ 0_{1\times(n-3)} & \sin\theta_2 & 0 & \cos\theta_2 \end{pmatrix}.$$

If we consider θ_2 such that

$$\bar{f}^n{}_{n-2}\cos\theta_2 = \bar{f}^n{}_n \sin\theta_2 \quad \Leftrightarrow \quad \mathrm{tg}\,\theta_2 = \frac{\bar{f}^n{}_{n-2}}{\bar{f}^n{}_n} = \frac{f^n{}_{n-2}}{f^n{}_{n-1}\sin\theta_1 + f^n{}_n\cos\theta_1},$$

then, the element $(n; n-2)$ of the matrix $F_2 = F_1 {}^tR_2$ is equal to 0. Since the component $(n; n-1)$ of F_1 is equal to 0, and as R_2 acts only on the $(n-2)$-th and n-th columns of F_1, the element $(n; n-1)$ of F_2 is also equal to 0. Writing then $F_2 = (\bar{\bar{f}}^i{}_j)^n_{i,j=1}$ and considering the matrix

$$R_3 = \begin{pmatrix} I_{n-4} & 0_{(n-4)\times 1} & 0_{(n-4)\times 2} & 0_{(n-4)\times 1} \\ 0_{1\times(n-4)} & \cos\theta_3 & 0_{1\times 2} & -\sin\theta_3 \\ 0_{2\times(n-4)} & 0_{2\times 1} & I_2 & 0_{2\times 1} \\ 0_{1\times(n-4)} & \sin\theta_3 & 0_{1\times 2} & \cos\theta_3 \end{pmatrix},$$

where $\mathrm{tg}\,\theta_3 = \frac{\bar{\bar{f}}^n{}_{n-3}}{\bar{\bar{f}}^n{}_n}$, we obtain a matrix $F_3 = F_2 {}^tR_3$ such that its components $(n; n-3)$, $(n; n-2)$ and $(n; n-1)$ are equal to zero. Continuing the same procedure with R_4, $R_5,\ldots$, till R_{n-2}, defining at the i-th step $F_i = F_{i-1} {}^tR_i$, we finally obtain the matrix :

$$F_{n-2} = \begin{pmatrix} \check{f}^1{}_1 & \check{f}^1{}_2 & \cdots & \check{f}^1{}_{n-1} & \check{f}^1{}_n \\ \check{f}^2{}_1 & \check{f}^2{}_2 & \cdots & \check{f}^2{}_{n-1} & \check{f}^2{}_n \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \check{f}^{n-1}{}_1 & \check{f}^{n-1}{}_2 & \cdots & \check{f}^{n-1}{}_{n-1} & \check{f}^{n-1}{}_n \\ \check{f}^n{}_1 & 0 & \cdots & 0 & \check{f}^n{}_n \end{pmatrix}.$$

Now, let F_{n-1} be the matrix such that $F_{n-2} = F_{n-1} R_{n-1}$, where :

$$R_{n-1} = \begin{pmatrix} \cos\theta_{n-1} & 0_{1\times(n-2)} & -\sin\theta_{n-1} \\ 0_{(n-2)\times 1} & I_{n-2} & 0_{(n-2)\times 1} \\ \sin\theta_{n-1} & 0_{1\times(n-2)} & \cos\theta_{n-1} \end{pmatrix}.$$

Then :

$$F_{n-1} = \begin{pmatrix} \tilde{f}^1{}_1\cos\theta_{n-1} - \tilde{f}^1{}_n\sin\theta_{n-1} & \tilde{f}^1{}_2 & \cdots & \tilde{f}^1{}_1\sin\theta_{n-1} + \tilde{f}^1{}_n\cos\theta_{n-1} \\ \tilde{f}^2{}_1\cos\theta_{n-1} - \tilde{f}^2{}_n\sin\theta_{n-1} & \tilde{f}^2{}_2 & \cdots & \tilde{f}^2{}_1\sin\theta_{n-1} + \tilde{f}^2{}_n\cos\theta_{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{f}^n{}_1\cos\theta_{n-1} - \tilde{f}^n{}_n\sin\theta_{n-1} & 0 & \cdots & \tilde{f}^n{}_1\sin\theta_{n-1} + \tilde{f}^n{}_n\cos\theta_{n-1} \end{pmatrix}.$$

The element $(n;1)$ of this matrix is equal to 0 when $\operatorname{tg}\theta_{n-1} = \frac{\tilde{\tilde{f}}^n_1}{\tilde{\tilde{f}}^n_n}$, that is when :

$$\theta_{n-1} = \operatorname{arctg}\left(\frac{\tilde{\tilde{f}}^n_1}{\tilde{\tilde{f}}^n_n}\right) + k\pi \;, \quad k \in \mathbb{Z} \;.$$

Thus, the component $(n;n)$ of F_{n-1} is :

$$\frac{\tilde{\tilde{f}}^n_n}{\cos\theta_{n-1}} \quad ;$$

it can be chosen either positive or negative (for any angle α, $\cos(\alpha + \pi) = -\cos\alpha$); but it never vanishes. Indeed, as ${}^tF\,F = I_n$, then :

$$
\begin{aligned}
{}^tF_{n-1}\,F_{n-1} &= {}^t(F\,{}^tR_1\,{}^tR_2\,\ldots\,{}^tR_{n-1})\,F\,{}^tR_1\,{}^tR_2\,\ldots\,{}^tR_{n-1} = \\
&= R_{n-1}\,\ldots\,R_2\,R_1\,{}^tF\,F\,{}^tR_1\,{}^tR_2\,\ldots\,{}^tR_{n-1} = \\
&= R_{n-1}\,\ldots\,R_2\,R_1\,{}^tR_1\,{}^tR_2\,\ldots\,{}^tR_{n-1} = I_n \;,
\end{aligned}
$$

and also :

$$
{}^tF_{n-1}\,F_{n-1} = I_n \quad\Leftrightarrow\quad F_{n-1}\,{}^tF_{n-1}\,F_{n-1} = F_{n-1} \quad\Leftrightarrow\quad F_{n-1}\,{}^tF_{n-1} = I_n \;;
$$

F_{n-1} and ${}^tF_{n-1}$ are both orthogonal matrices. Thus, we have :

$$\sum_{k,l=1}^{n} \delta^{kl}\,\tilde{\tilde{f}}^i_k\,\tilde{\tilde{f}}^j_l = \delta^{ij} \;, \tag{4.1.2}$$

where δ^{ij} is the component $(i;j)$ of the identity matrix I_n. For $i = j = n$, this relation becomes :

$$\sum_{k=1}^{n} \tilde{\tilde{f}}^n_k\,\tilde{\tilde{f}}^n_k = 1 \;.$$

Since $\tilde{\tilde{f}}^n_k = 0$ for all $1 \leqslant k \leqslant n-1$, then :

$$\tilde{\tilde{f}}^n_n\,\tilde{\tilde{f}}^n_n = 1 \;,$$

hence :

$$\tilde{\tilde{f}}^n_n = \pm 1 \neq 0 \;.$$

Note that for $j = n$ and $1 \leqslant i \leqslant n-1$, relation 4.1.2 is :

$$\sum_{k=1}^{n} \tilde{\tilde{f}}^i_k\,\tilde{\tilde{f}}^n_k = \delta^{in} \quad\Leftrightarrow\quad \tilde{\tilde{f}}^i_n\,\tilde{\tilde{f}}^n_n = \delta^{in} \;,$$

and shows that $\tilde{\tilde{f}}^i_n = 0$ for all $1 \leqslant i \leqslant n-1$. Thus, we arrive at the conclusion that the matrix F_{n-1} has the form :

$$F_{n-1} = \left(\begin{array}{c|c} F_{\text{small}} & 0 \\ \hline 0 & 1 \end{array}\right) \;,$$

where $F_{\text{small}} \in \mathrm{O}_{n-1}(\mathbb{R})$. Note that the matrices R_1, R_2, $\ldots$, R_{n-1} should be, respectively, written as $R_{n-1,n}$, $R_{n-2,n}$, $\ldots$, R_{1-n}, in order to have the same notation as used in the theorem.

The reasoning done above holds for any $n \geqslant 2$. The only place where n appears is in the number of steps. The argument can then also be applied to F_{small}; after $n-2$ steps, we obtain :

$$
F_{2n-3} = \left(\begin{array}{c|c} F_{\text{wee}} & 0 \\ \hline 0 & I_2 \end{array} \right) ,
$$

where $F_{\text{wee}} \in \mathrm{O}_{n-2}(\mathbb{R})$. Just note that in the calculation for obtaining F_{2n-3}, the multiplication of F_{n-1} by the matrix $R_{i,n-1} \in \mathrm{O}_n(\mathbb{R})$ is equivalent to the multiplication of F_{small} by the corresponding matrix $R_{i,n-1} \in \mathrm{O}_{n-1}(\mathbb{R})$.

Continuing this procedure till the ς-th step, where $\varsigma = \left(\frac{n}{2}(n-1) - 1 \right)$, we finally obtain the following expression :

$$
F = F_\varsigma \, R_\varsigma \, \ldots \, R_3 \, R_2 \, R_1 ,
$$

where the R_i matrices correspond to matrices $R_{ab}(\theta^{ab})$ which are arranged in a precise order, and :

$$
F_\varsigma = \left(\begin{array}{ccc} \hat{f}^1{}_1 & \hat{f}^1{}_2 & 0_{1\times(n-2)} \\ \hat{f}^2{}_1 & \hat{f}^2{}_2 & 0_{1\times(n-2)} \\ 0_{(n-2)\times 1} & 0_{(n-2)\times 1} & I_{n-2} \end{array} \right) .
$$

Let $R = R_{12}(\theta^{12})$. Then $F_\varsigma \, {}^t R$ is an orthogonal matrix the component $(2;1)$ of which is equal to zero if $\mathrm{tg}\,\theta^{12} = \frac{\hat{f}^2{}_1}{\hat{f}^2{}_2}$. As in the case of θ_{n-1} (see above), θ^{12} can be chosen in such a way that $\hat{f}^2{}_2 > 0$. As $F_\varsigma \, {}^t R \in \mathrm{O}_n(\mathbb{R})$, then $\hat{f}^2{}_2 = 1$ and $\hat{f}^1{}_2 = 0$. Thus, $\hat{f}^1{}_1$ is necessarily equal either to $+1$ or to -1. Hence, $F_\varsigma \, {}^t R = E$, where $E \in \{\mathrm{diag}(1; 1; 1; \ldots; 1) ; \, \mathrm{diag}(-1; 1; 1; \ldots; 1)\}$. We finally obtain the expression :

$$
F = E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\theta^{ab}) ,
$$

in which the matrices $R_{ab}(\theta^{ab})$ are arranged in a precise order. ∎

4.1.2 Remark : As the determinant of any $R_{ab}(\theta^{ab})$ is equal to $+1$, then $\det F = \det E$. Thus, if $\det F = +1$, then $E = I_n$, if $\det F = -1$, then $E = \mathrm{diag}(-1; 1; \ldots; 1)$.

4.1.3 Corollary : $\mathrm{O}_n(\mathbb{R})$ *is the union of the two disjoint sets :*

$$
\mathrm{O}_n(\mathbb{R}) = \mathrm{O}_n(\mathbb{R})^+ \sqcup \mathrm{O}_n(\mathbb{R})^- ,
$$

where :

$$
\mathrm{O}_n(\mathbb{R})^+ = \{F \in \mathrm{O}_n(\mathbb{R}) \mid \det F = +1\} ,
$$

$$
\mathrm{O}_n(\mathbb{R})^- = \{F \in \mathrm{O}_n(\mathbb{R}) \mid \det F = -1\} .
$$

Proof : Any matrix $F \in O_n(\mathbb{R})$ can be written as :

$$F = E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\theta^{ab}) \ ,$$

where $R_{ab}(\theta^{ab})$ is a matrix of the form 4.1.1. Let us consider the following smooth curves :

$$
\begin{aligned}
c_{ab} : [0 \, ; 1] &\longrightarrow \quad \mathbb{R} \\
t &\longmapsto \quad c_{ab}(t) = \theta^{ab} \, t \ , \qquad \text{where } 1 \leqslant a < b \leqslant n \ .
\end{aligned}
$$

Then :

$$
\begin{aligned}
\Phi : [0 \, ; 1] &\longrightarrow \qquad O_n(\mathbb{R}) \\
t &\longmapsto \quad E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\theta^{ab} \, t)
\end{aligned}
$$

is a continuous curve in $O_n(\mathbb{R})$ linking E to F. Any two matrices $A, B \in O_n(\mathbb{R})$ which have both the same determinant, for instance $+1$, can then be written as :

$$
\begin{aligned}
A &= E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\theta^{ab}) \ , \\
B &= E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\eta^{ab}) \ ,
\end{aligned}
$$

where $E = I_n$ in this case. With such expressions, we can easily find two continuous curves linking $E = I_n$ to A and B; for instance :

$$
\begin{aligned}
\Phi_A : [0 \, ; 1] &\longrightarrow \qquad O_n(\mathbb{R}) \\
t &\longmapsto \quad E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\theta^{ab} \, t) \ ,
\end{aligned}
$$

$$
\begin{aligned}
\Phi_B : [0 \, ; 1] &\longrightarrow \qquad O_n(\mathbb{R}) \\
t &\longmapsto \quad E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\eta^{ab} \, t) \ .
\end{aligned}
$$

Then, the map $\bar{\Phi} : [0 \, ; 1] \to O_n(\mathbb{R})$, given by

$$\bar{\Phi}(s) = \begin{cases} \Phi_A(2\,s) & \text{if } 0 \leqslant s \leqslant \frac{1}{2} \\ \\ \Phi_B(2 - 2\,s) & \text{if } \frac{1}{2} \leqslant s \leqslant 1 \end{cases} \ ,$$

is a continuous curve linking A to B. This shows that the set $O_n(\mathbb{R})^+$ is connected by arc. It is maximal, in the sense that there does not exist any bigger set $\tilde{O}^+$ connected by arc, containing it. Indeed, for any matrix $F \in \tilde{O}^+$, there exists a continuous curve

linking it to $E = I_n$; thus F is in $O_n(\mathbb{R})^+$, hence $O_n(\mathbb{R})^+ = \tilde{O}^+$. The same argument applied to $O_n(\mathbb{R})^-$ shows that this set is also connected by arc and maximal. In the jargon of topology, a maximal connected set is called connected component. We then conclude that $O_n(\mathbb{R})^+$ and $O_n(\mathbb{R})^-$ are two connected components. They are disjoint because their intersection is empty. Indeed, there exists no matrix the determinant of which is at the same time $+1$ and -1. Moreover, there exists no continuous curve linking $O_n(\mathbb{R})^+$ to $O_n(\mathbb{R})^-$, because otherwise, by continuity of the determinant map, it would not be contained in $O_n(\mathbb{R})$. ∎

4.1.4 Corollary : *Let $F \in O_n(\mathbb{R})$. According to theorem 4.1.1, it can be written as :*

$$F = F(\theta^{12}; \ldots; \theta^{n-1,n}) = E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\theta^{ab}) \ .$$

where $R_{ab}(\theta^{ab})$ has the form 4.1.1 and E is either equal to I_n or to $\mathrm{diag}(-1; 1; \ldots; 1)$. Then $F \in \mathrm{GL}_n(\mathbb{Z})$, that is F contains only integer numbers, if and only if

$$\theta^{ab} \in \left\{0; \frac{\pi}{2}; \pi; \frac{3\pi}{2}\right\} \ , \quad \forall\ 1 \leqslant a < b \leqslant n \ .$$

Proof : We follow exactly the same path as in the proof of theorem 4.1.1, while adding the following comments :

1. As F is orthogonal, the n vectors formed by the n columns composing this matrix constitute an orthonormal basis. Since F is supposed to contain only integer numbers, each column contains nothing but zeroes, except a ± 1 at exactly one index value; and this ± 1 must be at another line in each column.

2. If we do a right multiplication of F by the first matrix ${}^t R_1$, we obtain a matrix F_1, the component $(n; n-1)$ of which is zero if and only if $f^n_{\ n-1} \cos\theta_1 - f^n_{\ n} \sin\theta_1 = 0$. As $f^n_{\ n-1}, f^n_{\ n} \in \{0; 1\}$ and $f^n_{\ n-1} \neq f^n_{\ n}$, then $\theta_1 \in \{0; \frac{\pi}{2}; \pi; \frac{3\pi}{2}\}$. Thus R_1, which corresponds, in the double-index notation, to $R_{n-1,n}(\theta^{n-1,n})$, contains only integer numbers.

3. Since F and R_1 contain only integer numbers, the matrix F_1 contains only integer numbers. By induction, we deduce that all further matrices F_2, F_3, etc, are composed of integer numbers only. ∎

4.1.5 Definition : *Let $F \in O_n(\mathbb{R})$ be the orthogonal matrix representing a linear isometry f. If $F \in O_n(\mathbb{R})^+$, then f is called a rotation; if $F \in O_n(\mathbb{R})^-$, then f is called roto-reflection.*

These designations are justified by the fact that in three dimensions, a matrix of determinant $+1$ corresponds to a rotation around a one-dimensional subspace which is called rotation axis, and a matrix of determinant -1 represents a combination of a rotation and a reflection through a mirror plane. Moreover, note that the matrix $\mathrm{diag}(-1; 1; \ldots; 1)$ can be seen as the representation of a reflection through the subspace (the hyperplane) of all vectors, the first component of which is zero.

4.1.6 Remark : 1 – The matrix of a linear isometry is first of determinant ± 1 and not necessarily orthogonal. In the previous definition, the notions of rotation and roto-reflection were defined in the frame of orthogonal matrices, because orthogonal bases were chosen for the study of linear isometries. These notions can naturally be extended to the set of all matrices of determinant ± 1 which represent linear isometries. Indeed, as any of these matrices is similar to an orthogonal matrix, we can say that the set of these matrices is also composed of two disjoint connected components.

2 – In crystallography, one often uses the notion of *roto-inversion* instead of roto-reflection. This is justified by the fact that in our three-dimensional space, in which a crystal exists, an inversion is represented by a matrix of determinant -1. Indeed, the matrix associated to an inversion operation is $-I_n$, where n is the dimension of the space. In any space of odd dimension, in particular in the three-dimensional Euclidean space, the determinant of $-I_n$ is negative. Roto-reflections and roto-inversions are then equivalent concepts, and any matrix of determinant -1 could be written as a product of rotations and the matrix $-I_n$. In any space of even dimension, however, the determinant of the matrix representing an inversion is equal to $+1$. Thus a roto-inversion, which is the composition of a rotation, that is a matrix of determinant $+1$, and an inversion, represented by a matrix of determinant $+1$ as well, is therefore also a rotation and not a roto-reflection. Thus, in order to have a definition independent of the dimension of the considered space, we keep the concept of roto-reflection.

4.1.2 Lie Algebra

Any orthogonal $n \times n$ matrix, be its determinant $+1$ or -1, depends on $\frac{n}{2}(n-1)$ real parameters. Thus, $O_n(\mathbb{R})$ can be seen as a smooth manifold of dimension $\frac{n}{2}(n-1)$, composed of two disjoint connected sets $O_n(\mathbb{R})^+$ and $O_n(\mathbb{R})^-$, parameterised, respectively, by the maps :

$$(\theta^{12}; \theta^{13}; ...; \theta^{n-1,n}) \longmapsto F(\theta^{12}; \theta^{13}; \ldots; \theta^{n-1,n}) = \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\theta^{ab}) \, ,$$

$$(\vartheta^{12}; \vartheta^{13}; ...; \vartheta^{n-1,n}) \longmapsto \bar{F}(\vartheta^{12}; \vartheta^{13}; \ldots; \vartheta^{n-1,n}) = E \prod_{1 \leqslant a < b \leqslant n} R_{ab}(\vartheta^{ab}) \, ,$$

where $E = \mathrm{diag}(-1; 1; \ldots; 1)$. It is then a Lie group. Keep in mind that $0 \leqslant \theta^{ab}, \vartheta^{ab} < 2\pi$, in order to have a real parameterisation, that is a one-to-one map.

Let F be a matrix as defined above; its derivative with respect to θ^{ab} at $\theta \doteqdot (\theta^{12}; \theta^{13}; \ldots; \theta^{n-1,n}) = (0; 0; \ldots; 0)$ is :

$$\left. \frac{\partial F}{\partial \theta^{ab}} \right|_{\theta=0} \doteqdot T^{ab} \, ,$$

where :

$$T^{ab} = \begin{pmatrix} 0_r & 0_{r\times 1} & 0_{r\times s} & 0_{r\times 1} & 0_{r\times t} \\ 0_{1\times r} & 0 & 0_{1\times s} & -1 & 0_{1\times t} \\ 0_{s\times r} & 0_{s\times 1} & 0_s & 0_{s\times 1} & 0_{s\times t} \\ 0_{1\times r} & 1 & 0_{1\times s} & 0 & 0_{1\times t} \\ 0_{t\times r} & 0_{t\times 1} & 0_{t\times s} & 0_{t\times 1} & 0_t \end{pmatrix} \, ,$$

with $r = a - 1$, $s = b - a - 1$ et $t = n - b$. The set $\{T^{ab} \mid 1 \leqslant a < b \leqslant n\}$ corresponds to the canonical basis of the tangent space of $O_n(\mathbb{R})$ at I_n. This space is not only a vector space but also an algebra; it is the Lie algebra associated with $O_n(\mathbb{R})$ and is noted $\mathfrak{o}_n(\mathbb{R})$. It is a closed space under the Lie bracket operation; we have :

$$[T_{ab}; T_{ac}] = T_{bc} \in \mathfrak{o}_n(\mathbb{R}) , \quad \forall a < b < c ,$$

$$[T_{ab}; T_{cd}] = 0_n \in \mathfrak{o}_n(\mathbb{R}) , \quad \forall a < b < c < d .$$

Thanks to this operation, we only need the $n - 1$ first matrices $T_{12}; \ldots, T_{1n}$; all other matrices forming the canonical basis of the tangent space of $O_n(\mathbb{R})$ at I_n can be deduced by means of the first relation above. The elements composing this canonical basis are called *generators* of the Lie algebra $\mathfrak{o}_n(\mathbb{R})$.

Let us consider any basis vector T_{ab} and multiply it by the real number θ^{ab}, $1 \leqslant a < b \leqslant n$. A simple calculation shows that :

$$\exp(\theta^{ab} T_{ab}) = R_{ab}(\theta^{ab}) .$$

Note that as $[T_{ab}; T_{ac}] \neq 0$, then $\exp(T_{ac}) \exp(T_{bc}) \neq \exp(T_{ac} + T_{bc})$.

4.1.7 Remark : Only $O_n(\mathbb{R})^+$ is a subgroup of $O_n(\mathbb{R})$. Indeed, the product of two orthogonal matrices of determinant $+1$ is an orthogonal matrix of determinant $+1$ as well, whereas the product of two orthogonal matrices of determinant -1 is an orthogonal matrix with determinant $+1$. Moreover, the neutral element I_n of $O_n(\mathbb{R})$ is in $O_n(\mathbb{R})^+$ and not in $O_n(\mathbb{R})^-$. Observe that $O_n(\mathbb{R})^+$ is often noted $SO_n(\mathbb{R})$.

$SO_n(\mathbb{R})$ is also by itself a manifold, hence a Lie group. Its tangent space at I_n is the same as that of $O_n(\mathbb{R})$. This means that $O_n(\mathbb{R})$ and $SO_n(\mathbb{R})$ have the same Lie algebra. This is in fact normal because the neutral element I_n of $O_n(\mathbb{R})$ is in the $O_n(\mathbb{R})^+$ component. Note that the exponential of the product of any generator with a real parameter always corresponds to a matrix of determinant $+1$. Furthermore, if we calculate the derivative with respect to ϑ^{ab}, with $1 \leqslant a < b \leqslant n$, of any matrix of $O_n(\mathbb{R})^-$ and take its value at $\vartheta = 0$, $\vartheta = (\vartheta^{12}; \ldots; \vartheta^{n-1,n})$, we obtain a set of matrices which span a vector space but not an algebra (it is not closed under the Lie bracket operation). One can then wonder why the Lie algebra of $SO_n(\mathbb{R})$ is also that of $O_n(\mathbb{R})$. One reason will be given while studying one-parameter subgroups of the orthogonal group.

4.1.3 One-parameter Subgroups

From appendix B and as seen in the case of the group of translations, a one-parameter subgroup in a Lie group is a smooth curve γ such that $\gamma(t_1 + t_2) = \gamma(t_1) \gamma(t_2)$, which corresponds to a maximal integral curve of the elements of the associated Lie algebra. In the case of the group $GL_n(\mathbb{R})$, the Lie exponential map, which carries elements of the Lie algebra to elements of the Lie group, corresponds to the usual exp map. Evidently, this also holds for any continuous subgroup of $GL_n(\mathbb{R})$.

4.1.8 Definition : The one-parameter subgroups in $O_n(\mathbb{R})^+ = SO_n(\mathbb{R})$ are :

$$
\begin{aligned}
\mathbb{R} &\longrightarrow \quad O_n(\mathbb{R}) \\
t &\longmapsto \quad \exp(t\,\Psi)\ ,
\end{aligned}
$$

where :

$$
\Psi = \sum_{1\leqslant a < b \leqslant n} \theta^{ab}\, T_{ab}\ , \tag{4.1.3}
$$

$\theta^{ab} \in \mathbb{R}$, for all $1 \leqslant a < b \leqslant n$.

This definition is in agreement with any intuitive idea of rotation or roto-reflection one might have. Indeed, referred to a certain orthonormal basis, any rotation around the subspace of dimension $n - 2$ spanned by all vectors, the first two components of which are equal to zero, is represented by the matrix $\exp(t\,T_{12}) \in O_n(\mathbb{R})$, where t is a real parameter corresponding to the angle of rotation. Then, a rotation of angle t around any subspace of dimension $n - 2$ is simply given by the matrix :

$$
U^{-1} \exp(t\,T_{12})\, U\ , \tag{4.1.4}
$$

where $U \in O_n(\mathbb{R})^+$ is the transformation matrix from the given orthonormal basis to any other one. If t is seen as a free real parameter, expression 4.1.4 gives the general form of a one-parameter subgroup of $O_n(\mathbb{R})^+$. As :

$$
\exp(t\,\Psi) = \sum_{k=0}^{\infty} \frac{(t\,\Psi)^k}{k!}\ ,
$$

then :

$$
U^{-1} \exp(t\,T_{12})\, U = \exp(t\,U^{-1}\,T_{12}\,U)\ .
$$

Since :

$$
{}^{t}T_{ab} = -T_{ab}\ , \quad \forall\, 1 \leqslant a < b \leqslant n\ ,
$$

then :

$$
{}^{t}\!\left(\sum_{1\leqslant a < b \leqslant n} \theta^{ab}\, T_{ab}\right) = -\sum_{1\leqslant a < b \leqslant n} \theta^{ab}\, T_{ab}\ ,
$$

and also :

$$
{}^{t}(U^{-1}\,T_{12}\,U) = {}^{t}U\, {}^{t}T_{12}\, {}^{t}(U^{-1}) = -U^{-1}\,T_{12}\,U\ .
$$

Thus, we can write :

$$
U^{-1}\,T_{12}\,U = \sum_{1\leqslant a < b \leqslant n} \theta^{ab}\, T_{ab}\ ,
$$

where $\theta^{ab} \in \mathbb{R}$, for all $1 \leqslant a < b \leqslant n$. We then conclude that any rotation of angle t can be written as the exponential of the product of the parameter t and an element of the Lie algebra of $O_n(\mathbb{R})$. Reciprocally, any matrix

$$
\exp\!\left(t \sum_{1\leqslant a < b \leqslant n} \theta^{ab}\, T_{ab}\right)\ , \tag{4.1.5}
$$

where $t \in \mathbb{R}$ is a parameter and the θ^{ab}, $1 \leqslant a < b \leqslant n$ are fixed real numbers, is a one-parameter orthogonal matrix of determinant $+1$. To see that it is orthogonal, we calculate its transpose matrix and find that it is equal to its inverse :

$$^{\mathrm{t}}\left[\exp\left(t \sum_{1 \leqslant a < b \leqslant n} \theta^{ab} \, T_{ab}\right)\right] \;=\; \exp\left(t \sum_{1 \leqslant a < b \leqslant n} \theta^{ab} \, {}^{\mathrm{t}}T_{ab}\right) \;=\; \exp\left(t \sum_{1 \leqslant a < b \leqslant n} \theta^{ab} \, (-T_{ab})\right) =$$

$$=\; \exp\left(-t \sum_{1 \leqslant a < b \leqslant n} \theta^{ab} \, T_{ab}\right) =$$

$$=\; \left[\exp\left(t \sum_{1 \leqslant a < b \leqslant n} \theta^{ab} \, T_{ab}\right)\right]^{-1} .$$

It is of determinant $+1$ because it corresponds to a smooth curve passing through the identity matrix I_n. Thus, any matrix of the form 4.1.5 is in $\mathrm{O}_n(\mathbb{R})^+$, and we conclude that one-parameter subgroups of $\mathrm{O}_n(\mathbb{R})^+$ are of the form 4.1.5.

Let us also discuss the case $\mathrm{O}_n(\mathbb{R})^-$. As mentioned previously, it is not a subgroup of $\mathrm{O}_n(\mathbb{R})$. Since any matrix of $\mathrm{O}_n(\mathbb{R})^-$ can be written as a product of a matrix $E = \mathrm{diag}(-1; 1; \ldots; 1)$ and a matrix of $\mathrm{O}_n(\mathbb{R})^+$, any curve in $\mathrm{O}_n(\mathbb{R})^-$ can be written as

$$E \exp(t \, \Psi) \; ,$$

where Ψ has the form 4.1.3. The expression above shows that $\{T_{ab} \mid 1 \leqslant a < b \leqslant n\}$ generates not only rotations, that is elements of $\mathrm{O}_n(\mathbb{R})^+$, but also roto-reflections, that is elements of $\mathrm{O}_n(\mathbb{R})^-$. Note that as $\mathrm{O}_n(\mathbb{R})^-$ is not a group, hence curves in $\mathrm{O}_n(\mathbb{R})^-$ are not one-parameter subgroups.

4.2 Lattice symmetry

Any point of a curve in $\mathrm{O}_n(\mathbb{R})$ corresponds to the matrix part of a certain Euclidean isometry which is in general not a symmetry operation of a lattice; it depends in fact on the value of the parameter, which depends itself on the geometry of the considered lattice. Our goal is first to obtain the general condition for an orthogonal matrix to be the matrix part of a symmetry operation of a given lattice. Then, writing such an orthogonal matrix as an element of a curve in $\mathrm{O}_n(\mathbb{R})$, we shall find the values of the parameter which are compatible with the shape of the lattice.

4.2.1 Orthogonal matrices and modules

Let us recall that in the n-dimensional Euclidean manifold, endowed with a natural coordinate system $u = (u^1; \ldots; u^n)$, any n-dimensional lattice Λ can be written as $\Lambda = \{B \, \lambda \mid \lambda \in \mathbb{Z}^n\}$, where $B \in \mathrm{GL}_n(\mathbb{R})$. Any of its symmetry operations is a Euclidean isometry ϕ, the matrix and translation parts of which are, respectively, F and s with

respect to the chosen coordinate system (F is orthogonal in the natural coordinate system; if a non-natural (but still not curved) coordinate system were selected, F would not be orthogonal any more but still of determinant ± 1). For such a symmetry operation ϕ, let q be the point with coordinates u_q, lying on the symmetry element of ϕ. Then, the coordinates of the image $\phi(q)$ of q are $u_q + w$, where $w \in \mathbb{R}^n$ is the intrinsic translation of ϕ. The representation of Λ in the tangent spaces at q and $\phi(q)$ are :

$$\Upsilon_q = \{ B\,\lambda - u_q \mid \lambda \in \mathbb{Z}^n \} \,,$$

$$\Upsilon_{\phi(q)} = \{ B\,\lambda - u_q - w \mid \lambda \in \mathbb{Z}^n \} \,.$$

In order to find the image of a vector in Υ_q, we use the differential map $\mathrm{d}\phi_q$ of ϕ at q. We have :

$$\mathrm{d}\phi_q : \begin{pmatrix} u_q \\ B\,\lambda - u_q \end{pmatrix} \longmapsto \begin{pmatrix} u_q + w \\ F\,(B\,\lambda - u_q) \end{pmatrix} \,.$$

As ϕ is supposed to be a symmetry operation of Λ, the differential map $\mathrm{d}\phi_q$ must carry elements of Υ_q to elements of $\Upsilon_{\phi(q)}$. Thus, the vector $F\,(B\,\lambda - u_q)$, $\lambda \in \mathbb{Z}^n$, can be written as $B\,\lambda' - u_q - w$, for a certain $\lambda' \in \mathbb{Z}^n$:

$$F\,(B\,\lambda - u_q) = B\,\lambda' - u_q - w \,. \tag{4.2.1}$$

Since F is orthogonal, it can be written as $P^{-1} U\,P$, where P, P^{-1} and U are all orthogonal and U have the form :

$$U = \left(\begin{array}{c|c} I_m & 0 \\ \hline 0 & \bar{U} \end{array} \right) \,, \qquad \bar{U} \in \mathrm{O}_{n-m}(\mathbb{R}) \,.$$

Equation 4.2.1 becomes then :

$$P^{-1} U\,P\,(B\,\lambda - u_q) = B\,\lambda' - u_q - w \quad \Leftrightarrow$$

$$\Leftrightarrow \quad U\,P\,(B\,\lambda - u_q) = P\,(B\,\lambda' - u_q - w) \,. \tag{4.2.2}$$

Let us now write, respectively, $P\,B\,\lambda$, $P\,B\,\lambda'$, $P\,u_q$ and $P\,w$ as :

$$P\,B\,\lambda = \begin{pmatrix} (P\,B\,\lambda)_\| \\ (P\,B\,\lambda)_\perp \end{pmatrix} \,, \quad P\,B\,\lambda' = \begin{pmatrix} (P\,B\,\lambda')_\| \\ (P\,B\,\lambda')_\perp \end{pmatrix} \,,$$

$$P\,u_q = \begin{pmatrix} (P\,u_q)_\| \\ (P\,u_q)_\perp \end{pmatrix} \,, \quad P\,w = \begin{pmatrix} (P\,w)_\| \\ (P\,w)_\perp \end{pmatrix} \,,$$

where the parallel part corresponds to the first m components and the perpendicular part to the last $n - m$. Since w is the intrinsic translation, it has only a parallel component, $(P\,w)_\perp$ is then equal to 0. Equation 4.2.2 can then be written as :

$$\begin{cases} (P\,B\,\lambda)_\| - (P\,u_q)_\| &= (P\,B\,\lambda')_\| - (P\,u_q)_\| - (P\,w)_\| \\[2mm] \bar{U}\,(P\,B\,\lambda)_\perp - \bar{U}\,(P\,u_q)_\perp &= (P\,B\,\lambda')_\perp - (P\,u_q)_\perp \end{cases} \tag{4.2.3}$$

From the first equation, we obtain :

$$\left(P\,w\right)_\parallel = \left(P\,B\,\lambda'\right)_\parallel - \left(P\,B\,\lambda\right)_\parallel = \left(P\,B\,(\lambda'-\lambda)\right)_\parallel , \tag{4.2.4}$$

hence :

$$P\,w = \begin{pmatrix} \left(P\,B\,(\lambda'-\lambda)\right)_\parallel \\ 0 \end{pmatrix} . \tag{4.2.5}$$

This expression shows that $P\,w$ is an element of the set $\{P\,B\,\lambda \mid \lambda \in \mathbb{Z}^n\}$ which corresponds to the lattice Λ turned by the matrix P. This implies that w is an element of Λ. Note that as $n-m$ components of $P\,w$ are equal to zero, w is contained in the hyperplane $\{P^{-1}\,v \mid v = (v^1; \ldots; v^m; 0; \ldots; 0),\ v^1, \ldots, v^m \in \mathbb{R}\}$. Let us also have a look at the second equation of system 4.2.3. As q is a point in the symmetry element of the operation ϕ, the component $(P\,u_q)_\perp$ will be transformed through $\bar{U}$ into itself. Thus, we have simply :

$$\bar{U}\,(P\,B\,\lambda)_\perp = (P\,B\,\lambda')_\perp .$$

The system 4.2.3 can then be written in the following form :

$$\left(\begin{array}{c|c} I_m & 0 \\ \hline 0 & \bar{U} \end{array}\right) \begin{pmatrix} (P\,B\,\lambda)_\parallel \\ (P\,B\,\lambda)_\perp \end{pmatrix} = \begin{pmatrix} (P\,B\,\lambda')_\parallel \\ (P\,B\,\lambda')_\perp \end{pmatrix} + \begin{pmatrix} (P\,B\,\lambda'')_\parallel \\ 0 \end{pmatrix} , \tag{4.2.6}$$

which can be compactly written as :

$$U\,P\,B\,\lambda = P\,B\,\lambda' + P\,B\,\lambda'' = P\,B\,(\lambda' + \lambda'') \tag{4.2.7}$$

where $\lambda, \lambda', \lambda'' \in \mathbb{Z}^n$, λ'' being under the constraint $(P\,B\,\lambda'')_\perp = 0$. We finally obtain :

$$P^{-1}U\,P\,B\,\lambda = F\,B\,\lambda = B\,(\lambda' + \lambda'') . \tag{4.2.8}$$

This relation shows that F must transform any element of the lattice Λ to another element of Λ. Using a coarse notation, we have :

$$F\,\Lambda = \Lambda \ ;$$

in this expression, Λ must be considered as a finite free $\mathbb{Z}$-module, the elements of which are vectors. Writing symbolically $\Lambda = B\,\mathbb{Z}^n$, we have :

$$F\,B\,\mathbb{Z}^n = B\,\mathbb{Z}^n , \tag{4.2.9}$$

hence :

$$B^{-1}F\,B\,\mathbb{Z}^n = \mathbb{Z}^n . \tag{4.2.10}$$

Thus, we have proven the following result.

4.2.1 Proposition : *Let $\mathbb{R}^n$ be the Euclidean manifold endowed with a natural coordinate system $u = (u^1; \ldots; u^n)$, and $\Lambda = \{B\,\lambda \mid \lambda \in \mathbb{Z}^n\}$, where $B \in \mathrm{GL}_n(\mathbb{R})$, a lattice in $\mathbb{R}^n$. Let also ϕ be a Euclidean isometry, the matrix part of which is $F \in \mathrm{O}_n(\mathbb{R})$, with respect to the natural coordinate system, and the intrinsic translation is w. Then, ϕ is a symmetry operation of Λ if and only if $B^{-1}F\,B$ is a matrix containing only integer numbers, that is $B^{-1}F\,B \in \mathrm{GL}_n(\mathbb{Z})$, and $w = B\,\lambda$, for a certain $\lambda \in \mathbb{Z}^n$.*

The set of all $n \times n$ matrices naturally appears as the Euclidean manifold $\mathbb{R}^{n^2}$ in which the subset of all matrices with integer numbers can be seen as a lattice Γ, and the subset $\tilde{O} \doteq \{B^{-1} F B \mid F \in \mathrm{O}_n(\mathbb{R})\}$ is a smooth submanifold of dimension $\frac{n}{2}(n-1)$ constituted of two connected components. Thus, finding the matrices $F \in \mathrm{O}_n(\mathbb{R})$ such that $B^{-1} F B$ contains only integer numbers amounts to looking for all points of Γ lying in the submanifold $\tilde{O}$.

4.2.2   Cubic Lattices

We start our investigations by considering the case where the matrix $B = I_n$. Then, the lattice Λ simply corresponds to $\mathbb{Z}^n$. Such a lattice is said to be *cubic*. This lattice, when seen in the tangent space at the origin, has the structure of a finite free $\mathbb{Z}$-module. A natural basis of this module is the canonical basis of the tangent space at the origin. Thus, all n copies of $\mathbb{Z}$ constituting $\mathbb{Z}^n$ are mutually orthogonal. The *cubic* denomination derives from the fact that in the three-dimensional case, the parallelepiped generated by the three canonical basis vectors of the tangent space at the origin corresponds to a cube.

Before getting to the heart of the matter, some additional properties of one-parameter subgroups of $\mathrm{O}_n(\mathbb{R})$ need to be presented. Let us consider any matrix Ψ of the form 4.1.3. Then, $t \mapsto \exp(t\,\Psi)$ is a one-parameter subgroup in $\mathrm{O}_n(\mathbb{R})$, and if the coefficients θ^{ab} are chosen in such a way that $\Psi = U^{-1} T_{12}\, U$, for a certain orthogonal matrix U, then $\exp(t\,\Psi) = \exp(t\, U^{-1}\, T_{12}\, U) = U^{-1} \exp(t\, T_{12})\, U$ and t can be interpreted as a rotation angle. Indeed, $\exp(t\,\Psi)$ is a rotation matrix (it is of determinant $+1$), and when $t = 2\,\pi$, we have $\exp(2\,\pi\,\Psi) = U^{-1} \exp(2\,\pi\, T_{12})\, U = U^{-1} I_n\, U = I_n$. Thus, for any $t = 2\,\pi\, k$, $k \in \mathbb{Z}$, $\exp(t\,\Psi) = I_n$. Note that the set $\{t\,\Psi \mid t \in \mathbb{R}\}$ is a subspace of dimension one in $\mathfrak{o}_n(\mathbb{R})$; it is then an additive group isomorphic to $(\mathbb{R}; +)$. Furthermore, the set $\{\exp(t\,\Psi) \mid t \in \mathbb{R}\}$ is a group with respect to matrix multiplication, as $\exp\big((t_1 + t_2)\,\Psi\big) = \exp(t_1\,\Psi)\exp(t_2\,\Psi)$; we then obtain the following result.

4.2.2 Proposition : *The exponential map :*

$$
\begin{array}{cccc}
\exp : & \{t\,\Psi \mid t \in \mathbb{R}\} & \longrightarrow & \{\exp(t\,\Psi) \mid t \in \mathbb{R}\} \\
 & t\,\Psi & \longmapsto & \exp(t\,\Psi)
\end{array}
$$

is a group homomorphism. Its kernel, which is the set of all $t \in \mathbb{R}$ such that $\exp(t\,\Psi) = I_n$, is $\ker(\exp) = \{2\,\pi\, k\,\Psi \mid k \in \mathbb{Z}\}$. Thus, using the isomorphism theorem*, we have :*

$$
\{t\,\Psi \mid t \in \mathbb{R}\}/\ker(\exp) \cong \mathrm{Im}(\exp)\ ,
$$

where $\mathrm{Im}(\exp) = \{\exp(t\,\Psi) \mid t \in [0\,;\, 2\,\pi[\,\}$ *is the image of* exp.

This result is fundamental because it shows that only the values of t in the interval $[0\,;\, 2\,\pi[$ need to be considered.

4.2.3 Notation : As the parameter t corresponds to an angle of rotation, it will henceforth be noted α, a symbol commonly used for an angle.

The difficulty of finding the matrix part of symmetry operations of a cubic lattice increases with its dimension n. Indeed, the higher the dimension, the bigger the number of one-parameter subgroups in the group of orthogonal matrices. We shall therefore separately treat the cases $n = 2$, $n = 3$, in which some very important results for the usual crystallography will be obtained, and $n > 3$. Note that the case $n = 1$ does not need to be considered as $\mathrm{O}_1(\mathbb{R})$ contains only two matrices $I_1 = 1$ and $-I_1 = -1$ which correspond respectively to the identity and inversion operations.

Square lattice $(n = 2)$:
The Lie algebra $\mathfrak{o}_2(\mathbb{R})$ of $\mathrm{O}_2(\mathbb{R})$ is a vector space of dimension 1, it contains only one generator, which is :

$$T = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} . \tag{4.2.11}$$

Any one-parameter subgroup in $\mathrm{O}_2(\mathbb{R})$ is then given by $\alpha \mapsto \exp(\alpha\, T)$, where the parameter α corresponds to the angle of rotation. According to theorem 4.1.1, any matrix $F \in \mathrm{O}_2(\mathbb{R})$ with determinant $+1$ is indeed an element of this subgroup; the connected component of $\mathrm{O}_2(\mathbb{R})$ which contains the identity I_2 corresponds to this one-parameter subgroup, while the other one, that containing $E = \mathrm{diag}(-1;\, 1)$, is the set of all matrices $E \exp(\alpha\, T)$. Thus, any matrix $F \in \mathrm{O}_2(\mathbb{R})$ can be written as :

$$F = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \quad \text{if} \quad \det F = +1\,, \tag{4.2.12}$$

$$F = \begin{pmatrix} -\cos\alpha & \sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \quad \text{if} \quad \det F = -1\,, \tag{4.2.13}$$

where $\alpha \in [0\,;\, 2\,\pi[$. Such a matrix contains only integer numbers if and only if $\cos\alpha$ and $\sin\alpha$ are both integers, that is if and only if

$$\alpha \in \left\{ 0\,;\, \frac{\pi}{2}\,;\, \pi\,;\, \frac{3\,\pi}{2} \right\} .$$

With these values, we obtain the eight symmetry operations of a square, four rotations and four roto-reflections, given by the matrices :

$$\left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} ;\, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} ;\, \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} ;\, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right\}$$

and :

$$\left\{ \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} ;\, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} ;\, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} ;\, \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \right\} .$$

The first set contains the rotations of angle 0 (which corresponds to the identity matrix I_2), $\frac{\pi}{2}$, π and $\frac{3\pi}{2}$, while the second one contains the reflections through the mirror lines (which are one-dimensional vector subspaces) given, respectively, by

$$\{(0;\, a) \mid a \in \mathbb{R}\} \quad , \quad \{(a;\, a) \mid a \in \mathbb{R}\}\,,$$

$$\{(a;\, 0) \mid a \in \mathbb{R}\} \quad \text{and} \quad \{(a;\, -a) \mid a \in \mathbb{R}\}\,.$$

Note that the set of all these eight matrices form a group which is called the *point group of the square lattice.*

Cubic lattice $(n = 3)$:

This case is particularly interesting because the components of any vector in the Lie algebra $\mathfrak{o}_3(\mathbb{R})$ of $O_3(\mathbb{R})$ correspond to those of a vector characterising the axis of rotation. To see that, let us first write the generators of $\mathfrak{o}_3(\mathbb{R})$; we have :

$$T_{12} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} , \quad T_{13} = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} , \quad T_{23} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} . \quad (4.2.14)$$

As $\mathfrak{o}_3(\mathbb{R})$ is a (three-dimensional) vector space, we can consider as a basis any set of three linearly independent matrices, for instance $\{T_1; T_2; T_3\}$, where $T_1 = T_{23}$, $T_2 = -T_{13}$ and $T_3 = T_{12}$. It differs from that consisting of T_{12}, T_{13} and T_{23} only by the fact that T_{13} is replaced by $-T_{13}$; in this way, the relation $[T_1; T_2] = T_3$ holds for any cyclic permutation of 1, 2 and 3, without that a minus sign appears. Any vector Ψ of $\mathfrak{o}_3(\mathbb{R})$ can be written as :

$$\Psi = \sum_{j=1}^{3} \eta^j \, T_j , \quad \eta^j \in \mathbb{R} , \quad \forall \, 1 \leqslant j \leqslant 3 , \quad (4.2.15)$$

and any one-parameter subgroup of $O_3(\mathbb{R})$ is given by $t \mapsto \exp(t \, \Psi)$, where $t \in \mathbb{R}$. Let us focus on the particular subgroup $\alpha \mapsto \exp(\alpha \, T_1)$, where the parameter t is replaced by α. Using the power series of the exponential, we obtain :

$$\exp(\alpha \, T_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\alpha & -\sin\alpha \\ 0 & \sin\alpha & \cos\alpha \end{pmatrix} ;$$

it corresponds to a rotation of angle α around e_1, where e_1 is the first vector of the orthonormal basis $\{e_1; e_2; e_3\}$ of a three-dimensional vector space V furnished with a scalar product. To be precise, this matrix is in fact the matrix part of an isometry of the three-dimensional Euclidean manifold endowed with a natural coordinate system; the vector space V introduced here, with the orthonormal basis $\{e_1; e_2; e_3\}$, simply corresponds to a tangent space of the manifold, with its canonical basis (which is orthonormal).

Let $U = U_1 \, U_2$ be an orthogonal matrix, where :

$$U_1 = \begin{pmatrix} \cos\beta_1 & -\sin\beta_1 & 0 \\ \sin\beta_1 & \cos\beta_1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad \text{and} \quad U_2 = \begin{pmatrix} \cos\beta_2 & 0 & \sin\beta_2 \\ 0 & 1 & 0 \\ -\sin\beta_2 & 0 & \cos\beta_2 \end{pmatrix} .$$

Then $U^{-1} \exp(\alpha \, T_1) \, U$ corresponds to a rotation of angle α around the subspace

$$\mathcal{N} = \{v = U^{-1}w \mid w = (a; 0; 0), \, a \in \mathbb{R}\} ,$$

where the components of w are given with respect to the basis $\{e_1; e_2; e_3\}$. Indeed, the invariant vectors v through this map are given by

$$U^{-1} \exp(\alpha \, T_1) \, U \, v = v \quad \Leftrightarrow \quad \exp(\alpha \, T_1) \, U \, v = U \, v .$$

As $\beta_1, \beta_2 \in [0\,;\,2\pi[$, we see that v can have any orientation with respect to the basis vectors e_1, e_2 and e_3. Notice that $U^{-1} \exp(\alpha\,T_1)\,U = \exp(\alpha\,U^{-1}\,T_1\,U)$. If we calculate explicitly $U^{-1}\,T_1\,U$, with $U = U_1\,U_2$, we obtain :

$$U^{-1}\,T_1\,U = \begin{pmatrix} 0 & -\cos\beta_1\sin\beta_2 & -\sin\beta_1 \\ \cos\beta_1\sin\beta_2 & 0 & -\cos\beta_1\cos\beta_2 \\ \sin\beta_1 & \cos\beta_1\cos\beta_2 & 0 \end{pmatrix}\,,$$

which is antisymmetric, therefore an element of $\mathfrak{o}_3(\mathbb{R})$. It can then be written as :

$$U^{-1}\,T_1\,U = \sum_{j=1}^{3} \eta^j\,T_j\,,$$

where :

$$\begin{pmatrix} \eta^1 \\ \eta^2 \\ \eta^3 \end{pmatrix} = \begin{pmatrix} -\cos\beta_1\cos\beta_2 \\ \sin\beta_1 \\ -\cos\beta_1\sin\beta_2 \end{pmatrix}\,.$$

Writing η for the column-vector formed by η^1, η^2 and η^3, we see that

$$\eta = U^{-1}\,\zeta\,, \quad \text{where} \quad \zeta = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}\,.$$

If we think of η as a vector of V, with components η^1, η^2 and η^3 with respect to the orthonormal basis $\{e_1;\,e_2;\,e_3\}$, we see that it is an element of the subspace $\mathcal{N}$, the rotation axis of $U^{-1}\exp(\alpha\,T_1)\,U$. With this result, we conclude that any one-parameter subgroup $\alpha \mapsto \exp(\alpha\,\Psi)$ in $O_3(\mathbb{R})$, where $\Psi = \sum_{j=1}^{3} \eta^j\,T_j$, corresponds to a rotation of angle α around the axis generated by the unit vector $\eta = \sum_{j=1}^{3} \eta^j\,e_j$. Note that as $U, U^{-1} \in O_3(\mathbb{R})$ and as the norm of ζ is equal to one, then η is a unit vector, too. If we considered a non-unit vector $\vartheta = (\vartheta^1;\,\vartheta^2;\,\vartheta^3)$, then $\exp(\alpha\,\Psi)$, with $\Psi = \sum_{j=1}^{3} \theta^j\,T_j$, would also be the matrix of a rotation around the subspace generated by $\theta = \sum_{j=1}^{3} \vartheta^j\,e_j$, but the real angle of rotation would be $\alpha\,\|\vartheta\|$, where $\|\vartheta\|$ is the norm of ϑ. Indeed, $\alpha\sum_{j=1}^{3} \vartheta^j\,T_j = \alpha\,\|\vartheta\|\sum_{j=1}^{3} \frac{\vartheta^j}{\|\vartheta\|}\,T_j$, and we arrive at the case treated just above.

Let us find the explicit form of $\exp(\alpha\,\psi)$. For that, we need to calculate the powers of Ψ. We have :

$$\Psi = \begin{pmatrix} 0 & -\eta^3 & \eta^2 \\ \eta^3 & 0 & -\eta^1 \\ -\eta^2 & \eta^1 & 0 \end{pmatrix}\,, \tag{4.2.16}$$

$$\Psi^2 = \begin{pmatrix} -\eta^2\,\eta^2 - \eta^3\,\eta^3 & \eta^1\,\eta^2 & \eta^1\,\eta^3 \\ \eta^1\,\eta^2 & -\eta^1\,\eta^1 - \eta^3\,\eta^3 & \eta^2\,\eta^3 \\ \eta^1\,\eta^3 & \eta^2\,\eta^3 & -\eta^1\,\eta^1 - \eta^2\,\eta^2 \end{pmatrix}\,,$$

and :

$$\Psi^3 \;=\; -\|\eta\|^2 \begin{pmatrix} 0 & -\eta^3 & \eta^2 \\ \eta^3 & 0 & -\eta^1 \\ -\eta^2 & \eta^1 & 0 \end{pmatrix} \,,$$

$$\Psi^4 \;=\; -\|\eta\|^2 \begin{pmatrix} -\eta^2\,\eta^2 - \eta^3\,\eta^3 & \eta^1\,\eta^2 & \eta^1\,\eta^3 \\ \eta^1\,\eta^2 & -\eta^1\,\eta^1 - \eta^3\,\eta^3 & \eta^2\,\eta^3 \\ \eta^1\,\eta^3 & \eta^2\,\eta^3 & -\eta^1\,\eta^1 - \eta^2\,\eta^2 \end{pmatrix} \,.$$

Taking into account the fact that $\|\eta\| = 1$, we then obtain the two relations :

$$\begin{cases} \Psi^{2k+1} &=\; (-1)^k\,\Psi \\ \Psi^{2k+2} &=\; (-1)^k\,\Psi^2 \end{cases} \,, \qquad k \geqslant 0 \,.$$

Thus :

$$\exp(\alpha\,\Psi) \;=\; \sum_{k\geqslant 0} \frac{(\alpha\,\Psi)^k}{k!} \;=\; I_3 + \sum_{k\geqslant 0} \frac{(\alpha\,\Psi)^{2k+1}}{(2k+1)!} + \sum_{k\geqslant 0} \frac{(\alpha\,\Psi)^{2k+2}}{(2k+2)!} =$$

$$=\; I_3 + \sum_{k\geqslant 0} \frac{\alpha^{2k+1}}{(2k+1)!}\,(-1)^k\,\Psi + \sum_{k\geqslant 0} \frac{\alpha^{2k+2}}{(2k+2)!}\,(-1)^k\,\Psi^2 =$$

$$=\; I_3 + \sum_{k\geqslant 0}(-1)^k\,\frac{\alpha^{2k+1}}{(2k+1)!}\,\Psi - \sum_{k\geqslant 1}(-1)^k\,\frac{\alpha^{2k}}{(2k)!}\,\Psi^2 =$$

$$=\; I_3 + \Psi\,\sin\alpha + \Psi^2\,(1 - \cos\alpha) \,. \tag{4.2.17}$$

Explicitly :

$$\exp(\alpha\,\Psi) = \begin{pmatrix} f^1{}_1 & f^1{}_2 & f^1{}_3 \\ f^2{}_1 & f^2{}_2 & f^2{}_3 \\ f^3{}_1 & f^3{}_2 & f^3{}_3 \end{pmatrix} \,, \tag{4.2.18}$$

where :

$$\begin{cases} f^1{}_1 &=\; 1 - (1 - \cos\alpha)(\eta^2\,\eta^2 + \eta^3\,\eta^3) \\ f^1{}_2 &=\; -\eta^3\,\sin\alpha + \eta^1\eta^2\,(1 - \cos\alpha) \\ f^1{}_3 &=\; \eta^2\,\sin\alpha + \eta^1\,\eta^3\,(1 - \cos\alpha) \\[4pt] f^2{}_1 &=\; \eta^3\,\sin\alpha + \eta^1\,\eta^2\,(1 - \cos\alpha) \\ f^2{}_2 &=\; 1 - (1 - \cos\alpha)(\eta^1\,\eta^1 + \eta^3\,\eta^3) \\ f^2{}_3 &=\; -\eta^1\,\sin\alpha + \eta^2\,\eta^3\,(1 - \cos\alpha) \\[4pt] f^3{}_1 &=\; -\eta^2\,\sin\alpha + \eta^1\,\eta^3\,(1 - \cos\alpha) \\ f^3{}_2 &=\; \eta^1\,\sin\alpha + \eta^2\,\eta^3\,(1 - \cos\alpha) \\ f^3{}_3 &=\; 1 - (1 - \cos\alpha)(\eta^1\,\eta^1 + \eta^2\,\eta^2) \end{cases} \,. \tag{4.2.19}$$

We then conclude that any matrix $F \in O_3(\mathbb{R})$ depending on one parameter can be written as $E \exp(\alpha \Psi)$, where $\exp(\alpha \Psi)$ is given in expressions 4.2.18 and 4.2.19, and E is either equal to I_3 or to $\mathrm{diag}(-1; 1; 1)$. Our goal is to find the values of η^1, η^2, η^3 and α such that $\exp(\alpha \Psi)$ contain only integer numbers. For that, note first that, according to corollary 4.1.4, any matrix $F \in O_3(\mathbb{R})$ composed of only integer numbers can be written as :

$$ F = E \, R_{23}(\theta^{23}) \, R_{13}(\theta^{13}) \, R_{12}(\theta^{12}) \ , $$

where $\theta^{12}, \theta^{13}, \theta^{23} \in \{0 \, ; \, \frac{\pi}{2} \, ; \, \pi \, ; \, \frac{3\pi}{2}\}$. Let $O_3(\mathbb{Z})$ be the set of all such matrices; note that it is a subgroup of $O_3(\mathbb{R})$. The fact that any $F \in O_3(\mathbb{Z})$ depends on three parameters which can take only four different values each, shows that $O_3(\mathbb{Z})$ contains a finite number of elements. We then conclude that $O_3(\mathbb{Z})$ is a finite group. Thus, according to a famous result of the theory of finite groups, for any element g of a finite group $(\mathcal{G}; \diamond)$ (where $\diamond$ is the internal composition operation), there exists a natural number $N \in \mathbb{N} \smallsetminus \{0\}$ such that

$$ \underbrace{g \diamond \cdots \diamond g}_{N} = e \ , $$

where e is the neutral element in $\mathcal{G}$. In the present case, this means that for any matrix $F \in O_3(\mathbb{Z})$, there exists an $N \in \mathbb{N} \smallsetminus \{0\}$ such that $F^N = I_3$. As we are considering matrices F of the form $E \exp(\alpha \Psi)$, the condition is :

$$ F^N = \big(E \exp(\alpha \Psi)\big)^N = I_3 \ . \tag{4.2.20} $$

Let us first consider matrices F with determinant $+1$. Then, $E = I_3$, and :

$$ F^N = \exp(\alpha \Psi)^N = \exp(N \, \alpha \, \Psi) = I_3 \ . \tag{4.2.21} $$

This relation shows that :

$$ N \, \alpha = 2 \, \pi \, k \ , \quad k \in \mathbb{Z} \ , \tag{4.2.22} $$

with $\alpha \in [0 \, ; \, 2\,\pi[$, according to the isomorphism theorem. Thus, we have the following cases.

- $N = 1$, hence $\alpha = 0$. Then :

$$ \exp(0 \, \Psi) = \exp(0_3) = I_3 \ ; $$

  we obtain the identity matrix which contains of course only integer numbers.

- $N = 2$, hence $\alpha \in \{0 \, ; \, \pi\}$. If $\alpha = 0$, we have the case above. Let us consider $\alpha = \pi$. Then $\sin \alpha = 0$ and $\cos \alpha = -1$. Thus :

$$ \exp(\pi \, \Psi) = \begin{pmatrix} 1 - 2\,(\eta^2\,\eta^2 + \eta^3\,\eta^3) & 2\,\eta^1\,\eta^2 & 2\,\eta^1\,\eta^3 \\ 2\,\eta^1\,\eta^2 & 1 - 2\,(\eta^1\,\eta^1 + \eta^3\,\eta^3) & 2\,\eta^2\,\eta^3 \\ 2\,\eta^1\,\eta^3 & 2\,\eta^2\,\eta^3 & 1 - 2\,(\eta^1\,\eta^1 + \eta^2\,\eta^2) \end{pmatrix} . $$

  All the components of this matrix are integer numbers in the cases where $\eta^2 = \eta^3 = 0$ and then $\eta^1 = 1$ (η is a unit vector), $\eta^1 = \eta^3 = 0$ and $\eta^2 = 1$, and

$\eta^1 = \eta^2 = 0$ and $\eta^3 = 1$. Suppose now that only $\eta^3 = 0$. Then, the element $(1;1)$ of the matrix above becomes $1 - 2\,\eta^2\,\eta^2$. For this to be integer, we must have $\eta^2\,\eta^2 = \frac{m}{2}$, where $m \in \mathbb{N} \setminus \{0\}$. In fact, m must be equal to 1 because otherwise e^1 would necessarily be equal to zero, as η is a unit vector, or the norm of η would be bigger then one, which is not possible. Thus $\eta^2\,\eta^2 = \frac{1}{2}$. Using the same argument with the component $(2;2)$ of the matrix, we obtain $\eta^1\,\eta^1 = \frac{1}{2}$. In the same way, we find the two other cases $\eta^2 = 0$ and $\eta^1\,\eta^1 = \eta^3\,\eta^3 = \frac{1}{2}$, and $\eta^1 = 0$ and $\eta^2\,\eta^2 = \eta^3\,\eta^3 = \frac{1}{2}$. Finally, suppose that all components of η are different from zero. Then, from the component $(1;1)$, we obtain $\eta^1\,\eta^1 + \eta^2\,\eta^2 = \frac{m}{2}$, where $m \in \mathbb{N}$, hence $\eta^3\,\eta^3 = 1 - \frac{m}{2}$, as η is a unit vector. In fact, m must be equal to one, because otherwise at least one of the component of η would be equal to zero. Thus, $\eta^3\,\eta^3 = \frac{1}{2}$. Considering then the element $(2;2)$, we must have $\eta^1\,\eta^1 + \eta^3\,\eta^3 = \frac{m'}{2}$, where $m' \in \mathbb{N}$. Since $\eta^3\,\eta^3 = \frac{1}{2}$, we have $\eta^1\,\eta^1 = \frac{m'-1}{2}$. In this expression, $m' = 2$, otherwise one of the components of η would be equal to zero. Thus, we obtain $\eta^1\,\eta^1 = \eta^3\,\eta^3 = \frac{1}{2}$, implying that $\eta^2 = 0$, which is inconsistent with the hypothesis that all components of η are not equal to zero. We conclude that this last case is not possible. In short, we obtain nine rotations of angle π around the axes spanned by the unit vectors :

$$\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} ; \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} ; \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} ; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \\ 0 \end{pmatrix} ; \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ \pm 1 \end{pmatrix} ; \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ \pm 1 \end{pmatrix} \right\} .$$

The corresponding matrices are respectively :

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} , \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} , \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} ,$$

$$\begin{pmatrix} 0 & \pm 1 & 0 \\ \pm 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} , \quad \begin{pmatrix} 0 & 0 & \pm 1 \\ 0 & -1 & 0 \\ \pm 1 & 0 & 0 \end{pmatrix} , \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & \pm 1 \\ 0 & \pm 1 & 0 \end{pmatrix} .$$

- $N = 3$, hence $\alpha \in \{0 ; \frac{2\pi}{3} ; \frac{4\pi}{3}\}$. Again, in the case $\alpha = 0$, we obtain the identity matrix. Let us consider $\alpha = \frac{2\pi}{3}$. Then $\sin\alpha = \frac{\sqrt{3}}{2}$, $\cos\alpha = \frac{1}{2}$, and :

$$\exp(\tfrac{2\pi}{3}\,\Psi) = \begin{pmatrix} 1 - \frac{3}{2}(\eta^2\,\eta^2 + \eta^3\,\eta^3) & -\frac{\sqrt{3}}{2}\,\eta^3 + \frac{3}{2}\,\eta^1\,\eta^2 & \frac{\sqrt{3}}{2}\,\eta^2 + \frac{3}{2}\,\eta^1\,\eta^3 \\ \frac{\sqrt{3}}{2}\,\eta^3 + \frac{3}{2}\,\eta^1\,\eta^2 & 1 - \frac{3}{2}(\eta^1\,\eta^1 + \eta^3\,\eta^3) & -\frac{\sqrt{3}}{2}\,\eta^1 + \frac{3}{2}\,\eta^2\,\eta^3 \\ -\frac{\sqrt{3}}{2}\,\eta^2 + \frac{3}{2}\,\eta^1\,\eta^3 & \frac{\sqrt{3}}{2}\,\eta^1 + \frac{3}{2}\,\eta^2\,\eta^3 & 1 - \frac{3}{2}(\eta^1\,\eta^1 + \eta^2\,\eta^2) \end{pmatrix} .$$

We immediately see that $\eta^1 = 1$ and $\eta^2 = \eta^3$ is not possible : the components of the matrix are not integer. The same with $\eta^2 = 1$ and $\eta^1 = \eta^3 = 0$, and $\eta^3 = 1$

and $\eta^1 = \eta^2 = 0$. If only $\eta^3 = 0$, we obtain, considering the elements $(1;1)$ and $(2;2)$, $\eta^2 \eta^2 = \frac{2m}{3}$ and $\eta^1 \eta^1 = \frac{2m'}{3}$ respectively, where $m, m' \in \mathbb{Z}$. We notice that no value of m and m' makes sense; either we obtain a value of the norm of η bigger than one, or one of the components e^1 and e^2, or both, are equal to zero. Let us then consider all components of η different from zero. From the component $(1;1)$, we obtain $\eta^2 \eta^2 + \eta^3 \eta^3 = \frac{2m}{3}$, where $m \in \mathbb{Z}$. Only $m = 1$ is consistent with our hypothesis. As η is a unit vector, we deduce that $\eta^1 \eta^1 = \frac{1}{3}$. Using the same argument with the elements $(2;2)$ and $(3;3)$, we obtain $\eta^1 \eta^1 = \eta^2 \eta^2 = \eta^3 \eta^3 = \frac{1}{3}$, implying that each component is equal to $\pm\frac{\sqrt{3}}{2}$. Introducing these values in the other components of the matrix above, we see that we obtain only integer numbers. In conclusion, we have four rotations of angle $\frac{3\pi}{2}$ around the axes spanned by the unit vectors :

$$\left\{ \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} ; \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} ; \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix} ; \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix} \right\} .$$

The corresponding matrices are respectively :

$$\begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} , \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix} , \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix} , \begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} .$$

In the case where $\alpha = \frac{4\pi}{3}$, we obtain the same four possibilities for η. The corresponding matrices are simply obtained by taking the square of each of the four matrices written above. We have :

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} , \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} , \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} , \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{pmatrix} .$$

- $N = 4$, hence $\alpha \in \{0 ; \frac{\pi}{2} ; \pi ; \frac{3\pi}{2}\}$. In the case where $\alpha = \frac{\pi}{2}$, we have :

$$\exp(\tfrac{\pi}{2} \Psi) = \begin{pmatrix} 1 - (\eta^2 \eta^2 + \eta^3 \eta^3) & -\eta^3 + \eta^1 \eta^2 & \eta^2 + \eta^1 \eta^3 \\ \eta^3 + \eta^1 \eta^2 & 1 - (\eta^1 \eta^1 + \eta^3 \eta^3) & -\eta^1 + \eta^2 \eta^3 \\ \eta^2 + \eta^1 \eta^3 & \eta^1 + \eta^2 \eta^3 & 1 - (\eta^1 \eta^1 + \eta^2 \eta^2) \end{pmatrix} .$$

From the component $(1;1)$, we obtain $\eta^2 \eta^2 + \eta^3 \eta^3 \in \{0 ; 1\}$. If it is equal to zero, then $\eta^1 \eta^1 = 1$, as η is a unit vector. With this value, all components of the matrix above are integer. If $\eta^2 \eta^2 + \eta^3 \eta^3 = 1$, then $\eta^1 \eta^1 = 0$. From the elements $(2;2)$ and $(3;3)$, we obtain either $\eta^2 \eta^2 = 0$ and $\eta^3 \eta^3 = 1$, or $\eta^2 \eta^2 = 1$ and $\eta^3 \eta^3 = 0$. In any of these cases, the matrix above contains only integer numbers. In conclusion, we have three rotations of angle $\frac{\pi}{2}$ around the axes spanned by the unit vectors :

$$\left\{ \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} ; \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} ; \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \right\} .$$

The corresponding matrices are respectively :

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \ , \quad \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} \ , \quad \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \ .$$

In the case where $\alpha = \frac{3\pi}{2}$, we obtain the same three possibilities for η. The corresponding matrices are obtained by taking the cube of the matrices above, or by inverting them. We have :

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \ , \quad \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} \ , \quad \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \ .$$

$\alpha = \pi$ corresponds to the case $N = 2$, already treated above.

- $N \geqslant 5$, hence $\alpha \in \{\frac{2\pi m}{N} \mid 1 \leqslant m \leqslant N\}$. For the value $\alpha = \frac{2\pi}{N}$, $\cos \alpha \in]0\,;1[$, hence $1 - \cos \alpha \in]0\,;1[$. Thus, in order to have only integer components, we should have for instance $\eta^2 \eta^2 + \eta^3 \eta^3 > 1$, which is not consistent with the fact that η is a unit vector. We conclude that rotations of angle $\alpha = \frac{2\pi}{N}$, where $N \geqslant 5$ are not possible in a three-dimensional cubic lattice. Multiples of α can lead to an integer matrix, but in fact only when their values correspond to one of the previous cases ($N \leqslant 4$).

Let us also discuss matrices of the form $E \exp(\alpha\,\Psi)$, where $E = \mathrm{diag}(-1;1;1)$ and α is a real parameter which also belongs to the interval $[0\,;2\pi[$ (as the corresponding one-parameter subgroup $\alpha \mapsto \exp(\alpha\,\Psi)$ needs to be defined only in this interval). The set of these matrices is not a group because the composition of two of them gives a matrix with determinant $+1$. This is in particular the case when composing such a matrix with itself. We can then write :

$$E \exp(\alpha\,\Psi)\, E \exp(\alpha\,\Psi) = \exp(\beta\,\tilde{\Psi}) \ , \tag{4.2.23}$$

where $\beta \in [0\,;2\pi[$ and $\Psi, \tilde{\Psi} \in \mathfrak{o}_3(\mathbb{R})$. If $E \exp(\alpha\,\Psi)$ transforms $\mathbb{Z}^3$ into itself, so must $\exp(\beta\,\tilde{\Psi})$. Note that, as $O_3(\mathbb{Z})$ is a finite group, there exists an $L \in \mathbb{N} \smallsetminus \{0\}$ such that :

$$\left(E \exp(\alpha\,\Psi)\right)^L = I_3 \ . \tag{4.2.24}$$

Since $\det I_3 = +1$, then L must necessarily be an integer number, $L = 2\,N$, where $N \in \mathbb{N} \smallsetminus \{0\}$, hence :

$$\left(E \exp(\alpha\,\Psi)\right)^{2N} = I_3 \quad \Leftrightarrow \quad \left(\left(E \exp(\alpha\,\Psi)\right)^2 \right)^N = I_3 \ , \tag{4.2.25}$$

for a certain $\beta \in [0\,;2\pi[$ and $\tilde{\Psi} \in \mathfrak{o}_3(\mathbb{R})$. We conclude that $\exp(\beta\,\tilde{\Psi})$ can be only one of the rotation matrices previously obtained. To determine the different possible values of α and Ψ (that is η) in order that $E \exp(\alpha\,\Psi) \in O_3(\mathbb{Z})$, we consider again the cases $N = 1, 2, 3, 4$.

- $N = 1$. Then :

$$\left(E \exp(\alpha \, \Psi)\right)^2 = I_3 \quad \Leftrightarrow \quad E \exp(\alpha \, \Psi) = \left(E \exp(\alpha \, \Psi)\right)^{-1} = {}^{\mathrm{t}}\!\left(E \exp(\alpha \, \Psi)\right) ,$$

as it is an orthogonal matrix. The concrete form of $E \exp(\alpha \, \Psi)$ is essentially the same at that given in expressions 4.2.18 and 4.2.19, the only difference is that the components $(1;1)$, $(1;2)$ and $1;3)$ are multiplied by -1. The relation above implies :

$$\begin{cases} 2 \, \eta^1 \, \eta^2 \, (1 - \cos \alpha) &= 0 \\ 2 \, \eta^1 \, \eta^2 \, (1 - \cos \alpha) &= 0 \\ 2 \, \eta^1 \sin \alpha &= 0 \end{cases} .$$

These equations are satisfied for any η if $\alpha = 0$, or for any α if $\eta^1 = 0$. Furthermore, to obtain a matrix with only integer numbers, the angle α can take only the values $0, \frac{\pi}{2}, \pi$ and $\frac{3\pi}{2}$. For $\alpha = 0$, it is clear. For $\alpha \neq 0$, we have $\eta^1 = 0$, hence $\eta^2 \, \eta^2 + \eta^3 \, \eta^3 = 1$, as η is a unit vector. This implies that $\cos \alpha$ in the element $(1;1)$ can be only equal to 0 or ± 1, hence the four values for α given above. With this result, we obtain from the elements $(2;2)$ and $(3;3)$ that either $\eta^2 \, \eta^2 = 1$ and $\eta^3 \, \eta^3 = 0$, or $\eta^2 \, \eta^2 = 0$ and $\eta^3 \, \eta^3 = 1$. With these values, all the components are integer. Finally note that in the case $\alpha = \pi$, η^1 can be different from 0; if it is still equal to 0, then we can have $\eta^2 \, \eta^2 = \eta^3 \, \eta^3 = \frac{1}{2}$. In short, we have fourteen different possibilities. If $\alpha = 0$, we obtain :

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} ,$$

which corresponds to a reflection through the mirror plane

$$\{(0; \, a^2; \, a^3) \mid a^2, a^3 \in \mathbb{R}\} .$$

If $\alpha = \frac{\pi}{2}$, we have four matrices :

$$\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \quad \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \quad \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} , \quad \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix} ,$$

corresponding, respectively, to reflections through the four mirror planes

$$\{(a^1; \, a^1; \, a^3) \mid a^1, a^3 \in \mathbb{R}\} ,$$

$$\{(a^1; \, -a^1; \, a^3) \mid a^1, a^3 \in \mathbb{R}\} ,$$

$$\{(a^1; \, a^2; \, a^1) \mid a^1, a^3 \in \mathbb{R}\} ,$$

$$\{(a^1; \, a^2; \, -a^1) \mid a^1, a^3 \in \mathbb{R}\} .$$

If $\alpha = \pi$, we have four matrices :

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} , \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} , \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} , \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} ,$$

corresponding, respectively, to reflections through the four mirror planes

$$\{(a^1; 0; a^3) \mid a^1, a^3 \in \mathbb{R}\} \quad,$$

$$\{(a^1; a^2; 0) \mid a^1, a^2 \in \mathbb{R}\} \quad,$$

$$\{(a^1; a^2; a^2) \mid a^1, a^2 \in \mathbb{R}\} \quad,$$

$$\{(a^1; a^2; -a^2) \mid a^1, a^2 \in \mathbb{R}\} \quad,$$

and also :

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad,$$

which represents the inversion operation. Finally, if $\alpha = \frac{3\pi}{2}$, we obtain the same four matrices as in the case $\alpha = \frac{\pi}{2}$.

- $N = 2$. Then :

$$\left(E \exp(\alpha\,\Psi)\right)^2 = \exp(\pi\,\Psi) \quad \Leftrightarrow \quad E \exp(\alpha\,\Psi) = {}^{\mathrm{t}}\!\left(E \exp(\alpha\,\Psi)\right) \exp(\pi\,\Psi)\,.$$
$$(4.2.26)$$

We have obtained two kinds of rotations of angle π, those around a main direction of the cube and those around the face diagonals. Let us first treat the main directions, in particular that given by the unit vector $(1; 0; 0)$. The relation above leads to the following system of equations :

$$\begin{cases} (1 - \cos\alpha)(\eta^2\,\eta^2 + \eta^3\,\eta^3) & = & 1 \\ (1 - \cos\alpha)(\eta^1\,\eta^1 + \eta^3\,\eta^3) & = & 1 \\ \eta^3 \sin\alpha & = & 0 \\ \eta^3 \sin\alpha & = & 0 \\ \eta^1\,\eta^3\,(1 - \cos\alpha) & = & 0 \\ \eta^3 \sin\alpha & = & 0 \\ \eta^2\,\eta^3\,(1 - \cos\alpha) & = & 0 \end{cases} \quad .$$

We immediately see that α must be equal to π, otherwise $\eta^1 = \eta^2 = \eta^3 = 0$, which is not possible as η is a unit vector; $\alpha = 0$ is not possible either, because it does not satisfy the two first equations. We then deduce that $\eta^2\,\eta^2 + \eta^3\,\eta^3 = \frac{1}{2}$ and $\eta^1\,\eta^1 + \eta^3\,\eta^3 = \frac{1}{2}$. Subtracting these two relations, we obtain $\eta^1\,\eta^1 - \eta^2\,\eta^2 = 0 \Leftrightarrow \eta^1 = \pm\eta^2$. Note that η^1, therefore η^2, cannot be equal to zero; if this were the case, $\eta^3\,\eta^3$ would be equal to one, which would not be consistent with the two first equations of the system. Thus, in order to satisfy the fifth and seventh equations, η^3 must be equal to 0, which implies that $\eta^1 = \pm\frac{1}{\sqrt{2}}$ and $\eta^2 = \pm\eta^1$. We obtain the matrices :

$$\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \,, \quad \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \,,$$

which correspond to a rotation of angle $\frac{\pi}{2}$ and $\frac{3\pi}{2}$ respectively, followed by a reflection through the mirror plane $\{(a^1;\, a^2;\, 0) \mid a^1, a^2 \in \mathbb{R}\}$. With the same argument applied to the rotations around the two other main directions, we obtain :

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

and :

$$\begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}.$$

The first two matrices correspond, respectively, to rotations of angles $\frac{\pi}{2}$ and $\frac{3\pi}{2}$ around the direction given by $(0;\, 1;\, 0)$, followed by the reflection through the mirror plane $\{(a^1;\, 0;\, a^3) \mid a^1, a^3 \in \mathbb{R}\}$, while the two last represent rotations with same angles, around the direction given by $(0;\, 0;\, 1)$, followed by a reflection through the plane $\{(0;\, a^2;\, a^3) \mid a^2, a^3 \in \mathbb{R}\}$.

Let us also treat rotations around face diagonals. Consider in particular the direction given by the unit vector $\frac{1}{\sqrt{2}}(1;\, 1;\, 0)$. Equation 4.2.26 leads to a system of nine equations, among which the following three :

$$\begin{cases} \eta^2 \sin\alpha &=& 0 \\ \eta^2\,\eta^3\,(1 - \cos\alpha) &=& 0 \\ (1 - \cos\alpha)(\eta^1\,\eta^1 + \eta^2\,\eta^2) &=& 1 \end{cases}$$

The third equation shows that $\alpha \neq 0$. If $\eta^2 \neq 0$, the first equations impose that $\alpha = \pi$; if $\eta^2 = 0$, then $\eta^1\,\eta^1 + \eta^3\,\eta^3 = 1$, which implies that $\alpha \in \{\frac{\pi}{2}\,;\, \pi\,;\, \frac{3\pi}{2}\}$, in order that the element $(2; 2)$ of $E \exp(\alpha\,\Psi)$ be integer. This implies that for $\alpha \in \{\frac{\pi}{2}\,;\, \frac{3\pi}{2}\}$, either $\eta^1 = \pm 1$ and $\eta^3 = 0$, or $\eta^1 = 0$ and $\eta^3 = \pm 1$. This last case is not possible because it does not satisfy the third relation of the system above. In any event, for $\alpha \in \{\frac{\pi}{2}\,;\, \frac{3\pi}{2}\}$, equation 4.2.26 has no solution. Indeed, equating the component $(3; 1)$ of $E \exp(\alpha\,\Psi)$ and $^{\mathrm{t}}\!\big(E \exp(\alpha\,\Psi)\big) \exp(\pi\,\Psi)$, we obtain $0 = \pm 1$, which is absurd. Finally, if $\alpha = \pi$, we obtain, when equating the component $(3; 1)$ of the two matrices, $\eta^1\,\eta^3 = \eta^2\,\eta^3$. If $\eta^3 \neq 0$, then $\eta^1 = \eta^2$; inserting this in the third equation of the system above, we obtain $\eta^1 = \eta^2 = \pm\frac{1}{2}$, hence $\eta^3 = \pm\frac{1}{\sqrt{2}}$; this values are, however, not possible because they do not provide integer components. If $\eta^3 = 0$, then necessarily $\eta^1\,\eta^1 + \eta^2\,\eta^2 = 1$, which is not consistent with the third equation of the system above. Thus, equation 4.2.26 has no solution providing integer components to $E \exp(\pi\,\Psi)$. Repeating the same argument with all other rotations around face diagonals, we obtain the same result, there is no solution. We conclude that there is no orthogonal matrix of determinant -1 and containing only integer numbers, such that composed with itself, gives a rotation of angle π around the face diagonals of the cube.

- $N = 3$. Then :

$$\bigl(E\exp(\alpha\,\Psi)\bigr)^2 = \exp(\tfrac{2\pi}{3}\,\Psi) \quad\Leftrightarrow\quad E\exp(\alpha\,\Psi) = {}^{\mathrm{t}}\bigl(E\exp(\alpha\,\Psi)\bigr)\exp(\tfrac{2\pi}{3}\,\Psi)\;.\quad(4.2.27)$$

Let us first consider the rotation of angle $\frac{2\pi}{3}$ around the space diagonal of the cube given by the unit vector $\frac{1}{\sqrt{3}}(1;\,1;\,1)$. From relation 4.2.27, we obtain in particular :

$$\begin{cases} (\eta^2 - \eta^1)\bigl(\sin\alpha + \eta^3\,(1-\cos\alpha)\bigr) &=& 0 \\ (\eta^2 + \eta^3)\bigl(\sin\alpha - \eta^1\,(1-\cos\alpha)\bigr) &=& 0 \\ (\eta^1 + \eta^3)\bigl(\sin\alpha - \eta^2\,(1-\cos\alpha)\bigr) &=& 0 \end{cases}.$$

A solution of this system is $-\eta^3 = \eta^1 = \eta^2 = \pm\frac{1}{\sqrt{3}}$. Then, in order to have integer components, $\alpha \in \{0\,;\,\frac{2\pi}{3}\,;\,\frac{4\pi}{3}\}$. For these values, equation 4.2.27 is satisfied, except for $\alpha = 0$. For both other values $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$, we obtain the same matrix :

$$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{pmatrix}.$$

It corresponds to a rotation of angle $\frac{4\pi}{3}$ around the space diagonal given by $\frac{1}{\sqrt{3}}(1;\,1;\,1)$, followed by an inversion. The square of this matrix represents a rotation of angle $\frac{2\pi}{3}$ around the same subspace. Its cube corresponds to the inversion operation and its fourth power gives the rotation of angle $\frac{4\pi}{3}$ around the space diagonal considered. Finally, its fifth power, which is also its inverse, hence its transpose, is :

$$\begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix}.$$

Let us now suppose now that $\eta^1 \neq \eta^2$, for instance. Then, necessarily $\eta^3 \neq -\eta^2$ or $\eta^3 \neq -\eta^1$ or both. Let us consider the case $\eta^3 \neq -\eta^2$ (the argument is the same for $\eta^3 \neq -\eta^1$). From the two first equations of the system above, we obtain :

$$\eta^3 = -\frac{\sin\alpha}{1-\cos\alpha} = -\eta^1\;.$$

Inserting this result in the component $(2;2)$ of the matrix $E\exp(\alpha\,\Psi)$, we find :

$$1 - (1-\cos\alpha)(\eta^1\,\eta^1 + \eta^3\,\eta^3) \;=\; 1 - (1-\cos\alpha)\frac{2\sin\alpha}{(1-\cos\alpha)^2} \;=$$

$$=\; 1 - \frac{2\sin^2\alpha}{1-\cos\alpha} \;=\; 1 - \frac{2\,(1-\cos^2\alpha)}{1-\cos\alpha} \;=$$

$$=\; 1 - 2\,(1+\cos\alpha) \;=\; -1 + 2\cos\alpha\;.$$

Since $E\exp(\alpha\,\Psi)$ is orthogonal, any of its element cannot be bigger than one. This condition, combined with the fact that the components must be integer numbers,

implies that $\alpha \in \{0\,;\,\frac{\pi}{3}\,;\,\frac{\pi}{2}\,;\,\frac{3\pi}{2}\,;\,\frac{5\pi}{3}\}$. The value $\alpha = 0$ is not possible because it does not satisfy equation 4.2.27. Angles $\alpha = \frac{\pi}{2}$ and $\alpha = \frac{3\pi}{2}$ are not possible either, because we would then have $\eta^1 = -\eta^3 = 1$, which is not consistent with the fact that η is a unit vector. Finally, $\alpha = \frac{\pi}{3}$ and $\alpha = \frac{5\pi}{3}$ are not possible either, because η^1 would be bigger than one. We conclude that there is no solution outside the condition $-\eta^3 = \eta^1 = \eta^2$. All this expansion can be repeated with rotations of angle $\frac{2\pi}{3}$ around the diagonals given by the unit vectors $\frac{1}{\sqrt{3}}(1;\,1;\,-1)$, $\frac{1}{\sqrt{3}}(1;\,-1;\,1)$ and $\frac{1}{\sqrt{3}}(1;\,-1;\,-1)$. We obtain, respectively :

$$\begin{pmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix},$$

their fifth powers (their inverses) are, respectively :

$$\begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 & -1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

- $N = 4$. Then :

$$\big(E\exp(\alpha\,\Psi)\big)^2 = \exp(\tfrac{\pi}{2}\,\Psi) \iff E\exp(\alpha\,\Psi) = {}^{\mathrm{t}}\big(E\exp(\alpha\,\Psi)\big)\exp(\tfrac{\pi}{2}\,\Psi)\,. \quad (4.2.28)$$

Let us consider the rotation of angle $\frac{\pi}{2}$ around the subspace given by the unit vector $(1;\,0;\,0)$. From relation 4.2.28, we have in particular :

$$\begin{cases} (\eta^2 - \eta^1)\big(\sin\alpha + \eta^3\,(1-\cos\alpha)\big) &=& 0 \\ (\eta^2 - \eta^1)\big(\sin\alpha - \eta^3\,(1-\cos\alpha)\big) &=& 0 \\ \eta^1\,\eta^3\,(1-\cos\alpha) &=& 0 \\ \eta^1\sin\alpha &=& 0 \end{cases}.$$

If $\alpha = 0$, equation 4.2.28 is not satisfied. From the fourth equation of the system, we have that either $\alpha = \pi$, or $\eta^1 = 0$, or both. Suppose that $\alpha = \pi$. Then the third equation implies that either $\eta^1 = 0$ or $\eta^3 = 0$. If $\eta^3 = 0$, then η^1, $\eta^2 \in \{0\,;\,\pm\frac{1}{\sqrt{2}}\,;\,\pm 1\}$. In order that the norm of η be one, we have either $\eta^1 = 0$ and $\eta^2 = \pm 1$, or $\eta^1 = \pm\frac{1}{\sqrt{2}}$ and $\eta^2 = \pm\frac{1}{\sqrt{2}}$, or $\eta^1 = \pm 1$ and $\eta^2 = 0$. However, all these possibilities lead to contradictions in expression 4.2.28. Suppose now that $\eta^3 \neq 0$. The third equation implies $\eta^1 = 0$ and the two first $\eta^2 = 0$. Thus, $\eta^3 = \pm 1$. When inserting these values into relation 4.2.28, we obtain contradictions. Finally, consider $\eta^1 = 0$. Adding the two first equations of the system, we obtain $\eta^2 \sin\alpha = 0$, from which we deduce that either $\eta^2 = 0$ or $\sin\alpha = 0$, or both. Suppose that $\eta^2 = 0$. Then $\eta^3 = \pm 1$ and $\alpha \in \{\frac{\pi}{2}\,;\,\pi\,;\,\frac{3\pi}{2}\}$, in order to have integer components in the matrix $E\exp(\alpha\,\Psi)$. However, none of these possibilities satisfies equation 4.2.28. If $\sin\alpha = 0$, then $\alpha = \pi$, $\alpha = 0$ is not possible. Thus, we have either $\eta^2 = 0$ and $\eta^3 = \pm 1$, $\eta^2 = \pm\frac{1}{\sqrt{2}}$ and $\eta^3 = \pm\frac{1}{\sqrt{2}}$, or $\eta^2 = \pm 1$ and $\eta^3 = 0$.

When inserting these values into expression 4.2.28, we obtain contradictions. We conclude that there is no orthogonal matrix of determinant -1 containing only integer numbers, such that its square gives a rotation of angle $\frac{\pi}{2}$ around the subspace given by $(1; 0; 0)$. Repeating the argument with the rotation of angle $\frac{\pi}{2}$ around the two other main directions, and also with the rotation of angle $\frac{3\pi}{2}$ around the main directions, we obtain no solution.

4.2.4 Remark : In three-dimensional crystallography, rotations of angle $\frac{2\pi}{N}$, with $N \in \mathbb{N} \smallsetminus \{0\}$, around a subspace of dimension one are called N-fold axes, and the subspace is called rotation axis. If such rotations are combined with a reflection, the mirror plane of which is normal to the axis, they are called $\bar{N}$-fold roto-reflection axes. Note that in three dimensions, the matrix representing the inversion operation is of determinant -1. Thus a rotation of angle α followed by an inversion can be expressed by a rotation (around the same axis) of an angle being a multiple of α, followed by a reflection (the mirror plane of which is normal to the axis).

All the calculations and derivations previously done are assuredly long and somewhat repetitive. However, they have a certain importance because they constitute an algebraic way of finding the matrix part of all isometries of a three-dimensional cubic lattice. Furthermore, it constitutes a proof of the following result :

4.2.5 Proposition : *A three-dimensional cubic lattice contains nothing but N- and $\bar{N}$-fold axes, where $N \in \{1; 2; 3; 4\}$. There is no axis of higher order.*

4.2.6 Remark : The set of all matrices $F \in O_3(\mathbb{Z})$, that is the set of all $F \in O_3(\mathbb{R})$ transforming a cubic lattice into itself, contains exactly 48 elements. This number can be found by simply counting the number of matrices obtained : the identity, nine rotations of angle π, four rotations of angle $\frac{2\pi}{3}$ and four of angle $\frac{4\pi}{3}$, three rotations of angle $\frac{\pi}{2}$ and three of angle $\frac{3\pi}{2}$, the inversion, nine mirrors, the three rotations of angle $\frac{\pi}{2}$ followed by the inversion, the three rotations of angle $\frac{3\pi}{2}$ followed by the inversion, the four rotations of angle $\frac{2\pi}{3}$ followed by the inversion, and finally the four rotations of angle $\frac{4\pi}{3}$ followed by the inversion. This total number can also be deduced from combinatorial calculus : any matrix $F \in O_3(\mathbb{Z})$ contains only zeroes in each column, except at exactly one position, there is a ± 1; in each column, the ± 1 must be at another line; we obtain then six different possibilities in the first column (three with $+1$ and three with -1), four possibilities in the second column (two with $+1$ and two with -1), and two in the third one ($+1$ or -1). The total number of possibilities is therefore $6 \cdot 4 \cdot 2 = 48$.

n-dimensional cubic lattice $(n > 3)$:
An explicit form of one-parameter subgroups of $O_n(\mathbb{R})$, $n > 3$ is much more difficult to obtain in this case. Indeed, for $n > 3$, the cube on any element $T \in \mathfrak{o}_n(\mathbb{R})$ is in general not equal to a multiple of the element itself. The calculation of the exponential becomes then difficult. Moreover, the components of T no longer correspond to the components of vectors spanning the subspace (of dimension $n - 2$) around which the

rotation is made. Thus, the best way for obtaining all the matrices $F \in \mathrm{O}_n(\mathbb{R})$, that is the orthogonal matrices transforming $\mathbb{Z}^n$ into itself, is to use corollary 4.1.4. Indeed, with this corollary, we are sure to find all the possibilities and we can classify them according to the four values $\{0 \,;\, \frac{\pi}{2} \,;\, \pi \,;\, \frac{3\pi}{2}\}$ that each parameter θ^{ab} can take. The two weak points of this process are first that different combinations of values of all the parameters θ^{ab}, $1 \leqslant a < b \leqslant n$ can lead to the same matrix, and second that it does not directly indicate the subspace around which a rotation is made. Finally note that all orthogonal matrices with only integer numbers can be obtained by considering that each column contains only zeros, except at one position there is a $+1$ or a -1; and this position must be different in each column. We thus obtain the $2n\,(2n-2)(2n-4)(2n-6)\ldots 2 = 2^n\,n!$ matrices constituting $\mathrm{O}_n(\mathbb{R})$.

4.2.3 Other Lattice Systems

All the work done for the n-dimensional cubic lattice can be extended to any lattice $\Lambda = \{B\,\lambda \mid \lambda \in \mathbb{Z}^n\} \subset \mathbb{R}^n$, as long as the explicit form of the matrix B is known. It is of course nonsense to try doing it for all possible matrices B. The goal of this subsection is rather to discuss the form of the matrix B according to the matrices $F \in \mathrm{O}_n(\mathbb{R})$ transforming the lattice Λ (seen as a $\mathbb{Z}$-module) into itself.

Let us first note that B can always have the form of an upper-triangular matrix, with all diagonal elements different from zero. Any basis can be obtained by distorting the canonical basis $\{(1;\,0;\,\ldots;\,0)\,;\,\ldots\,;\,(0;\,0;\,\ldots,\,1)\}$ through B and then rotating it through $U \in \mathrm{SO}_n(\mathbb{R})$ (or through $U \in \mathrm{O}_n(\mathbb{R})^-$ if a negative orientation is required); since U does not modify the shape of the obtained basis (it preserves the norms and angles), we only need to take account of the action of B. This procedure to obtain any basis is just the inverse operation of the *Gram-Schmidt process* for orthonormalising any basis in a vector space endowed with a scalar product. Note that only B with a positive determinant will be considered, in order to keep the orientation of the canonical basis.

It is important to realise that the connection between the form of the matrix B (*i.e.* the shape of the lattice) and the set of matrices F such that $B^{-1}F\,B \in$

Figure 4.1: Two different bases for describing the same two-dimensional square lattice.

$\mathrm{GL}_n(\mathbb{Z})$, is a tricky subject; concerning this, several remarks require particular attention.

1. The set of matrices transforming a lattice Λ into itself is intrinsic to Λ and not to the choice of a basis of Λ. Indeed, the shape of Λ does not change when choosing another basis. If we consider for instance the square lattice (in the two-dimensional Euclidean space), we see that $\{(1;\,0)\,;\,(0;\,1)\}$ and $\{(1;\,0)\,;\,(1;\,1)\}$ are both a basis for this same lattice; and the second one is obtained by the application of the

upper-triangular matrix

$$B = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

to the vectors of the first one. The lattices (seen here as a $\mathbb{Z}$-module) generated by the first and the second bases correspond to one and the same lattice Λ; hence the set of matrices F transforming Λ into itself is the same in both cases, the only difference lying in the fact that $F = I_2^{-1} F I_2$ is different from $B^{-1} F B$ (see figure 4.1). More generally, let us consider two lattices $\Lambda_1 = \{B_1 \lambda \mid \lambda \in \mathbb{Z}^n\}$ and $\Lambda_2 = \{B_2 \lambda \mid \lambda \in \mathbb{Z}^n\}$. Then, Λ_2 can be obtain from Λ_1 by applying the matrix B, given by $B B_1 = B_2$, to all elements of Λ_1. As the set of upper-triangular matrices form a group, we can assert that B is also upper-triangular. If all the components of B are integer and if the diagonal elements all have the value ± 1, then the two lattices are equal, and a unique basis can be chosen for both. Indeed, as all the diagonal elements of B are equal to ± 1, then $\det B = \pm 1$, hence the parallelepipeds spanned by each basis have equal volumes. These two lattices correspond to a unique one and the set of matrices $F \in O_n(\mathbb{R})$ transforming a lattice into itself is the same for Λ_1 and Λ_2.

2. We could then consider an equivalence relation of bases, saying that two bases are equivalent if the lattices they generate have the same set of matrices transforming them into themselves. However, this definition is not appropriate, as in one class, two bases generating two lattices with a different shape could be found. Indeed, if we take for instance the two lattices generated by the two bases $\{(2;\, 0)\,;\, (0;\, 1)\}$ and $\{2;\, 0)\,;\, (1;\, \frac{1}{2})\}$, we find that both have the same set of matrices F transforming them into themselves, while they do not have completely the same shape. In a way, these two lattices can be described from a same basis, for instance $\{(2;\, 0)\,;\, (0;\, 1)\}$, while specifying that the second one has a node in the centre of each square spanned by the two basis vectors. The two lattices have thus almost the same shape, but not completely. In general, all matrices B corresponding to a same lattice can be grouped in a class. Thus, the set of all B may be viewed as a set of classes. These classes can in turn be grouped into classes, or *superclasses*, according to the following criterion : two different classes are in a same superclass if and only if for any B_1 in the first class and B_2 in the second, $\{F \in O_n(\mathbb{R}) \mid B_1^{-1} F B_1 \in GL_n(\mathbb{R})\} = \{F \in O_n(\mathbb{R}) \mid B_2^{-1} F B_2 \in GL_n(\mathbb{R})\}$, that is both lattices $\Lambda_1 = \{B_1 \lambda \mid \lambda \in \mathbb{Z}^n\}$ and $\Lambda_2 = \{B_2 \lambda \mid \lambda \in \mathbb{Z}^n\}$, seen as $\mathbb{Z}$-modules, have the same set of matrices $F \in O_n(\mathbb{R})$ transforming them to themselves. Such a class of classes, or superclass, is called *crystal system*. More information may be found in the textbooks written by D. Schwarzenbach and G. Chapuis [SC06], and by W. Opechowski [ech86].

3. The shape of a lattice and the equality of two lattices are notions which must be considered with care. If two lattices are related through a scalar matrix $a\, I_n$, where $a \in \mathbb{R}^*$, the set of matrices $F \in O_n(\mathbb{R})$ transforming a lattice into itself is exactly the same for both of them, while $a\, I_n$ is an upper-triangular matrix which does not contain in general only integer numbers. Thus, in the previous point, we

could introduce one more class of classes, between the classes and the superclasses, according to the criterion : two classes are equivalent if and only if two matrices B_1 and B_2 can be found, B_1 in the first class and B_2 in the second, such that $B_1 = a\, B_2$, where $a \in \mathbb{R}^*$. Note that a is considered as positive, in order to keep positively oriented matrices.

4. Let $\Lambda_1 = \{B_1\, \lambda \mid \lambda \in \mathbb{Z}^n\}$ and $\Lambda_2 = \{B_2\, \lambda \mid \lambda \in \mathbb{Z}^n\}$ be two lattices, and $F \in O_n(\mathbb{R})$ a matrix such that $F\, \Lambda_1 = \Lambda_1$, that is F transforms Λ_1 into itself. Let B be a matrix given by $B\, B_1 = B_2$. If :

$$[F\,;\, B] = F\, B - B\, F = 0_n \,, \qquad (4.2.29)$$

then $F\, \Lambda_2 = \Lambda_2$, that is F transforms also Λ_2 into itself. The converse is not necessarily true. Indeed, if we take for instance two lattices in three dimensions, spanned by the two bases $\{(1;\, 0;\, 0);\, (0;\, 1;\, 0);\, (0;\, 0;\, 1)\}$ and $\{(1;\, 0;\, 0);\, (0;\, 1;\, 0);\, (\frac{1}{2};\, \frac{1}{2};\, \frac{1}{2})\}$, then the matrix F, corresponding to a rotation of angle $\frac{2\pi}{3}$ around the subspace spanned by the vector $\frac{1}{\sqrt{3}}(1;\, 1;\, 1)$, transforms each lattice into itself, while $[F\,;\, B] \neq 0$, where B is the matrix transforming one basis to another one.

Two-dimensional lattices :
In the two-dimensional Euclidean space, the angle of rotation transforming a lattice into itself can take only values $\frac{2\pi}{N}$, where $N \neq 5$ and $N \leqslant 6$, and their multiples. Indeed, let us consider any matrix $F \in SO_2(\mathbb{R})$ such that $F\, \Lambda = \Lambda$, where $\Lambda = \{B\, \lambda \mid \lambda \in \mathbb{Z}^2\}$. Then, $F\, B\, \lambda = B\, \lambda' \Leftrightarrow B^{-1}\, F\, B\, \lambda = \lambda'$, where $\lambda, \lambda' \in \mathbb{Z}^2$, hence $B^{-1}\, F\, B$ contains only integer numbers. Since the trace is a similarity constant, $\mathrm{Tr}(B^{-1}\, F\, B) = \mathrm{Tr}\, F$, we obtain :

$$2\cos\alpha = m \,, \quad \text{where } m \in \mathbb{Z} \,,$$

hence :

$$\alpha \in \left\{ 0\,;\, \frac{\pi}{3}\,;\, \frac{\pi}{2}\,;\, \frac{2\pi}{3}\,;\, \pi\,;\, \frac{4\pi}{3}\,;\, \frac{3\pi}{2}\,;\, \frac{5\pi}{3} \right\} \,.$$

As seen in the previous subsection, rotations of angle $\frac{\pi}{3}$, $\frac{2\pi}{3}$ do not appear in the square lattice. The question is to know if there exists indeed a lattice for which such rotations appear; and if it is the case, to be able to find its characteristics. To answer these points, we shall find the explicit form of the matrix $B^{-1}\, F\, B$, where $F \in SO_2(\mathbb{R})$. Let :

$$B = \begin{pmatrix} b^1{}_1 & b^1{}_2 \\ 0 & b^2{}_2 \end{pmatrix} \,, \qquad B^{-1} = \begin{pmatrix} \frac{1}{b^1{}_1} & -\frac{b^1{}_2}{b^1{}_1\, b^2{}_2} \\ 0 & \frac{1}{b^2{}_2} \end{pmatrix} \,. \qquad (4.2.30)$$

Then :

$$B^{-1} F B = \begin{pmatrix} \frac{1}{b^1{}_1} & -\frac{b^1{}_2}{b^1{}_1\, b^2{}_2} \\ 0 & \frac{1}{b^2{}_2} \end{pmatrix} \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \begin{pmatrix} b^1{}_1 & b^1{}_2 \\ 0 & b^2{}_2 \end{pmatrix} =$$

$$= \begin{pmatrix} \cos\alpha - \frac{b^1{}_2}{b^2{}_2}\sin\alpha & -\left(\frac{b^2{}_2}{b^1{}_1} + \frac{b^1{}_2\, b^1{}_2}{b^1{}_1\, b^2{}_2}\right)\sin\alpha \\ \frac{b^1{}_1}{b^2{}_2}\sin\alpha & \frac{b^1{}_2}{b^2{}_2}\sin\alpha + \cos\alpha \end{pmatrix} \,. \qquad (4.2.31)$$

In the case where $\alpha = \frac{\pi}{3}$, we obtain :

$$B^{-1}F\,B = \begin{pmatrix} \frac{1}{2} - \frac{\sqrt{3}\,b^1{}_2}{2\,b^2{}_2} & -\frac{\sqrt{3}}{2}\left(\frac{b^2{}_2}{b^1{}_1} + \frac{b^1{}_2\,b^1{}_2}{b^1{}_1\,b^2{}_2}\right) \\ \frac{\sqrt{3}\,b^1{}_1}{2\,b^2{}_2} & \frac{\sqrt{3}\,b^1{}_2}{2\,b^2{}_2} + \frac{1}{2} \end{pmatrix}\ . \qquad (4.2.32)$$

This matrix must contain only integer numbers. For the component $(2;1)$, we have :

$$b^2{}_2 = \frac{\sqrt{3}\,b^1{}_1}{2\,m_1}\ , \qquad \text{where } m_1 \in \mathbb{Z}\ .$$

For the component $(1;1)$, we have :

$$\frac{1}{2} - \frac{\sqrt{3}\,b^1{}_2}{2\,b^2{}_2} = m_2 \quad \Leftrightarrow \quad b^1{}_2 = \frac{2\,b^2{}_2}{\sqrt{3}}\left(\frac{1}{2} - m_2\right) = \frac{b^1{}_1}{m_1}\left(\frac{1}{2} - m_2\right)\ , \quad m_2 \in \mathbb{Z}\ .$$

Inserting this expression in the component $(2;2)$, we obtain an integer number. Let us have finally a look at the element $(1;2)$; we have :

$$-\frac{\sqrt{3}}{2}\left(\frac{b^2{}_2}{b^1{}_1} + \frac{b^1{}_2\,b^1{}_2}{b^1{}_1\,b^2{}_2}\right) = -\frac{3}{4\,m_1} - \left(\frac{1}{2} - m_2\right)^2\ .$$

We see that it is an integer number for several different values of m_1 and m_2. In fact, we observe that m_1 can only be equal to 1; in this case, m_2 may be any integer number. For any other value of m_1 (in particular $m_1 = -1$) there is no integer solution. Let us consider $m_1 = 1$ and $m_2 = 0$. The matrix B then adopts the form :

$$B = b^1{}_1 \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix}\ .$$

The corresponding lattice is shown in figure 4.2. Several bases can be considered, the two most common ones are repre-

Figure 4.2: Illustration of a two-dimensional lattice containing rotations of angle $\frac{\pi}{3}$. The two bases commonly used are represented with their corresponding two-dimensional parallelepipeds.

sented. The upper-left is obtained by applying B to the canonical vectors $(1;0)$ and $(0;1)$. The lower-right is obtained in the same way, by applying the matrix :

$$B = b^1{}_1 \begin{pmatrix} 1 & -\frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix}\ ,$$

which corresponds to the case $m_1 = m_2 = 1$.

If we repeat the same calculations for the case of a rotation of angle $\frac{2\pi}{3}$, we obtain exactly the same possibilities for B. Indeed, the matrix $B^{-1}F\,B$ is almost the same,
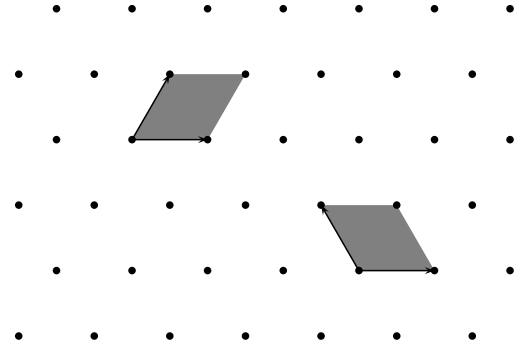
the only difference is that $\frac{1}{2}$ is replaced by $-\frac{1}{2}$ in the components $(1;1)$ and $(2;2)$. This shows that lattices containing rotations of angle $\frac{2\pi}{3}$ are always compatible with those containing rotations of angle $\frac{\pi}{3}$, in two dimensions. This kind of lattice is, of course, incompatible with the square one.

Any lattice in two dimensions contains at least rotations of angle π. Indeed, rotations of angle π are compatible with the square lattice and they are represented by the scalar matrix $-I_2$. As all scalar matrices commute with any other matrix, we conclude (using the fourth remark on page 115) that these rotations are compatible with any two-dimensional (Euclidean) lattice. Among all the lattices containing only rotations of angle π, two kinds may be distinguished, those containing reflections through mirror lines, and those which do not possess them. In the first case, the shape of a lattice is a parallelogram, while in the second case it must be a rectangle or a diamond. With these considerations, we obtain all the possible lattice systems in two-dimensions, mostly classified according to the angle of rotation. Three kinds can be considered; those containing rotations of angle $\frac{\pi}{3}$ and $\frac{2\pi}{3}$ (and not $\frac{\pi}{2}$), called *hexagonal* or *triangular*, those containing rotations of angle $\frac{\pi}{2}$ (and not $\frac{\pi}{3}$ or $\frac{2\pi}{3}$), called *square*, and finally those possessing rotations of angle π only. For this last case, we can distinguish lattices having mirror lines, called *rectangular* or with *diamond shape*, and those which do not contain them, called simply *oblique*. The typical matrices B corresponding to hexagonal or triangular, square, rectangular and oblique are respectively given by :

$$a\begin{pmatrix} 1 & \pm\frac{1}{2} \\ 0 & \frac{\sqrt{3}}{2} \end{pmatrix} \ , \quad \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} \ , \quad \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix} \ , \quad \begin{pmatrix} a & b \\ 0 & c \end{pmatrix} \ ,$$

where $a, b, c \in \mathbb{R}_+^*$. According to the second remark on page 114, lattices corresponding to these four matrices may be obtained from other ones having another form.

Three-dimensional lattices :

As in two dimensions, three-dimensional lattice can contain only rotations of angle $\frac{2\pi}{N}$, where $N = 1, 2, 3, 4$, and their multiples. Indeed, let us consider a matrix $F \in \mathrm{O}_3(\mathbb{R})$ transforming a lattice $\Lambda = \{B\,\lambda \mid \lambda \in \mathbb{Z}^3\}$ into itself. Then $B^{-1}F\,B$ contains only integer numbers; its trace is in particular integer. Since F can be written as $F = U^{-1}\bar{F}\,U$, where $U \in \mathrm{O}_3(\mathbb{R})$ and :

$$\bar{F} = \begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & \pm 1 \end{pmatrix} \ ,$$

and as the trace of a matrix is a similarity constant, $\mathrm{Tr}(B^{-1}F\,B) = \mathrm{Tr}(B^{-1}U^{-1}\bar{F}\,U\,B) = \mathrm{Tr}\,\bar{F}$, we obtain :

$$2\cos\alpha \pm 1 = m \ , \quad \text{where } m \in \mathbb{Z} \ ,$$

hence we obtain the same possible angles as in two dimensions. In the previous subsection, we have seen that rotations of angle $\frac{2\pi}{N}$, where $N > 4$, do not appear in the cubic lattice. One can wonder if there exists a lattice in three dimensions containing rotations of angle $\frac{\pi}{3}$. As it exists in two dimensions, we can immediately ascertain its validity in

three dimensions. To find its shape, we consider the general forms for B and B^{-1} :

$$B = \begin{pmatrix} b^1{}_1 & b^1{}_2 & b^1{}_3 \\ 0 & b^2{}_2 & b^2{}_3 \\ 0 & 0 & b^3{}_3 \end{pmatrix} \ , \quad B^{-1} = \begin{pmatrix} \frac{1}{b^1{}_1} & -\frac{b^1{}_2}{b^1{}_1 \, b^2{}_2} & \frac{b^1{}_2 \, b^2{}_3 - b^1{}_3 \, b^2{}_2}{b^1{}_1 \, b^2{}_2 \, b^3{}_3} \\ 0 & \frac{1}{b^2{}_2} & -\frac{b^2{}_3}{b^2{}_2 \, b^3{}_3} \\ 0 & 0 & \frac{1}{b^3{}_3} \end{pmatrix} \ . \tag{4.2.33}$$

Let $\alpha \mapsto \exp(\alpha \, \Psi)$, where $\exp(\alpha \, \Psi)$ has the explicit form given in expressions 4.2.17 and 4.2.16, be any one-parameter subgroup of $O_3(\mathbb{R})$. Then :

$$B^{-1} \exp(\alpha \, \Psi) \, B = I_3 + \sin \alpha \, B^{-1} \Psi \, B + (1 - \cos \alpha) \, B^{-1} \Psi^2 \, B \ , \tag{4.2.34}$$

where :

$$B^{-1} \Psi \, B = \begin{pmatrix} \bar{\psi}^1{}_1 & \bar{\psi}^1{}_2 & \bar{\psi}^1{}_3 \\ \bar{\psi}^2{}_1 & \bar{\psi}^2{}_2 & \bar{\psi}^2{}_3 \\ \bar{\psi}^3{}_1 & \bar{\psi}^3{}_2 & \bar{\psi}^3{}_3 \end{pmatrix} \ , \quad B^{-1} \Psi^2 \, B = \begin{pmatrix} \hat{\psi}^1{}_1 & \hat{\psi}^1{}_2 & \hat{\psi}^1{}_3 \\ \hat{\psi}^2{}_1 & \hat{\psi}^2{}_2 & \hat{\psi}^2{}_3 \\ \hat{\psi}^3{}_1 & \hat{\psi}^3{}_2 & \hat{\psi}^3{}_3 \end{pmatrix} \ , \tag{4.2.35}$$

with :

$$\begin{cases} \bar{\psi}^1{}_1 &= -\frac{b^1{}_2 \, \eta^3}{b^2{}_2} - \frac{(b^1{}_2 \, b^2{}_3 - b^1{}_3 \, b^2{}_2) \, \eta^2}{b^2{}_2 \, b^3{}_3} \\[2mm] \bar{\psi}^1{}_2 &= -\left(\frac{b^1{}_2 \, \eta^3}{b^1{}_1 \, b^2{}_2} + \frac{(b^1{}_2 \, b^2{}_3 - b^1{}_3 \, b^2{}_2) \, \eta^2}{b^1{}_1 \, b^2{}_2 \, b^3{}_3} \right) b^1{}_2 + \left(-\frac{\eta^3}{b^1{}_1} + \frac{(b^1{}_2 \, b^2{}_3 - b^1{}_3 \, b^2{}_2) \, \eta^1}{b^1{}_1 \, b^2{}_2 \, b^3{}_3} \right) b^2{}_2 \\[2mm] \bar{\psi}^1{}_3 &= -\left(\frac{b^1{}_2 \, \eta^3}{b^1{}_1 \, b^2{}_2} + \frac{(b^1{}_2 \, b^2{}_3 - b^1{}_3 \, b^2{}_2) \, \eta^2}{b^1{}_1 \, b^2{}_2 \, b^3{}_3} \right) b^1{}_3 + \left(-\frac{\eta^3}{b^1{}_1} + \frac{(b^1{}_2 \, b^2{}_3 - b^1{}_3 \, b^2{}_2) \, \eta^1}{b^1{}_1 \, b^2{}_2 \, b^3{}_3} \right) b^2{}_3 + \\[2mm] & \quad + \left(\frac{\eta^2}{b^1{}_1} + \frac{b^1{}_2 \, \eta^1}{b^1{}_1 \, b^2{}_2} \right) b^3{}_3 \\[2mm] \bar{\psi}^2{}_1 &= \left(\frac{\eta^3}{b^2{}_2} + \frac{b^2{}_3 \, \eta^2}{b^2{}_2 \, b^3{}_3} \right) b^1{}_1 \\[2mm] \bar{\psi}^2{}_2 &= \left(\frac{\eta^3}{b^2{}_2} + \frac{b^2{}_3 \, \eta^2}{b^2{}_2 \, b^3{}_3} \right) b^1{}_2 - \frac{b^2{}_3 \, \eta^1}{b^3{}_3} \\[2mm] \bar{\psi}^2{}_3 &= \left(\frac{\eta^3}{b^2{}_2} + \frac{b^2{}_3 \, \eta^2}{b^2{}_2 \, b^3{}_3} \right) b^1{}_3 - \frac{b^2{}_3 \, b^2{}_3 \, \eta^1}{b^2{}_2 \, b^3{}_3} - \frac{b^3{}_3 \, \eta^1}{b^2{}_2} \\[2mm] \bar{\psi}^3{}_1 &= -\frac{b^1{}_1 \, \eta^2}{b^3{}_3} \\[2mm] \bar{\psi}^3{}_2 &= -\frac{b^1{}_2 \, \eta^2}{b^3{}_3} + \frac{b^2{}_2 \, \eta^1}{b^3{}_3} \\[2mm] \bar{\psi}^3{}_3 &= -\frac{b^1{}_3 \, \eta^2}{b^3{}_3} + \frac{b^2{}_3 \, \eta^1}{b^3{}_3} \end{cases} \tag{4.2.36}$$

and :

$$
\left\{
\begin{aligned}
\hat{\psi}^1{}_1 &= -\eta^2\,\eta^2 - \eta^3\,\eta^3 - \frac{b^1{}_2\,\eta^1\,\eta^2}{b^2{}_2} - \frac{(b^1{}_2\,b^2{}_3 - b^1{}_3\,b^2{}_2)\,\eta^1\,\eta^3}{b^2{}_2\,b^3{}_3} \\
\hat{\psi}^1{}_2 &= -\left(\frac{\eta^2\,\eta^2 - \eta^3\,\eta^3}{b^1{}_1} + \frac{b^1{}_2\,\eta^1\,\eta^2}{b^1{}_1\,b^2{}_2} - \frac{(b^1{}_2\,b^2{}_3 - b^1{}_3\,b^2{}_2)\,\eta^1\,\eta^2}{b^1{}_1\,b^2{}_2\,b^3{}_3}\right) b^1{}_2 + \\
&\quad + \left(\frac{\eta^1\,\eta^2}{b^1{}_1} + \frac{b^1{}_2\,(\eta^1\,\eta^1 + \eta^3\,\eta^3)}{b^1{}_1\,b^2{}_2} + \frac{(b^1{}_2\,b^2{}_3 - b^1{}_3\,b^2{}_2)\,\eta^2\,\eta^3}{b^1{}_1\,b^2{}_2\,b^3{}_3}\right) b^2{}_2 \\
\hat{\psi}^1{}_3 &= -\left(\frac{\eta^2\,\eta^2 - \eta^3\,\eta^3}{b^1{}_1} + \frac{b^1{}_2\,\eta^1\,\eta^2}{b^1{}_1\,b^2{}_2} - \frac{(b^1{}_2\,b^2{}_3 - b^1{}_3\,b^2{}_2)\,\eta^1\,\eta^2}{b^1{}_1\,b^2{}_2\,b^3{}_3}\right) b^1{}_3 + \\
&\quad + \left(\frac{\eta^1\,\eta^2}{b^1{}_1} + \frac{b^1{}_2\,(\eta^1\,\eta^1 + \eta^3\,\eta^3)}{b^1{}_1\,b^2{}_2} + \frac{(b^1{}_2\,b^2{}_3 - b^1{}_3\,b^2{}_2)\,\eta^2\,\eta^3}{b^1{}_1\,b^2{}_2\,b^3{}_3}\right) b^2{}_3 + \\
&\quad + \left(\frac{\eta^1\,\eta^3}{b^1{}_1} - \frac{b^1{}_2\,\eta^2\,\eta^3}{b^1{}_1\,b^2{}_2} - \frac{(b^1{}_2\,b^2{}_3 - b^1{}_3\,b^2{}_2)(\eta^1\,\eta^1 + \eta^2\,\eta^2)}{b^1{}_1\,b^2{}_2\,b^3{}_3}\right) b^3{}_3 \\[4pt]
\hat{\psi}^2{}_1 &= \left(\frac{\eta^1\,\eta^2}{b^2{}_2} - \frac{b^2{}_3\,\eta^1\,\eta^3}{b^2{}_2\,b^3{}_3}\right) b^1{}_1 \\
\hat{\psi}^2{}_2 &= \left(\frac{\eta^1\,\eta^2}{b^2{}_2} - \frac{b^2{}_3\,\eta^1\,\eta^3}{b^2{}_2\,b^3{}_3}\right) b^1{}_2 - \left(\frac{\eta^1\,\eta^1 - \eta^3\,\eta^3}{b^2{}_2} + \frac{b^2{}_3\,\eta^2\,\eta^3}{b^2{}_2\,b^3{}_3}\right) b^2{}_2 \\
\hat{\psi}^2{}_3 &= \left(\frac{\eta^1\,\eta^2}{b^2{}_2} - \frac{b^2{}_3\,\eta^1\,\eta^3}{b^2{}_2\,b^3{}_3}\right) b^1{}_3 - \left(\frac{\eta^1\,\eta^1 - \eta^3\,\eta^3}{b^2{}_2} + \frac{b^2{}_3\,\eta^2\,\eta^3}{b^2{}_2\,b^3{}_3}\right) b^2{}_3 + \\
&\quad + \left(\frac{\eta^2\,\eta^3}{b^2{}_2} + \frac{b^2{}_3\,(\eta^1\,\eta^1 + \eta^2\,\eta^2)}{b^2{}_2\,b^3{}_3}\right) b^3{}_3 \\[4pt]
\hat{\psi}^3{}_1 &= \frac{b^1{}_1\,\eta^1\,\eta^3}{b^3{}_3} \\
\hat{\psi}^3{}_2 &= \frac{b^1{}_2\,\eta^1\,\eta^3}{b^3{}_3} + \frac{b^2{}_2\,\eta^2\,\eta^3}{b^3{}_3} \\
\hat{\psi}^3{}_3 &= \frac{b^1{}_3\,\eta^1\,\eta^3}{b^3{}_3} + \frac{b^2{}_3\,\eta^2\,\eta^3}{b^3{}_3} - \eta^1\,\eta^1 - \eta^2\,\eta^2
\end{aligned}
\right.
\tag{4.2.37}
$$

Let us consider $\alpha = \frac{\pi}{3}$. The component $(3;3)$ of $B^{-1} \exp(\frac{\pi}{3}\,\Psi)\,B$ is :

$$
1 + \frac{\sqrt{3}}{2}\left(-\frac{b^1{}_3\,\eta^2}{b^3{}_3} + \frac{b^2{}_3\,\eta^1}{b^3{}_3}\right) + \frac{1}{2}\left(\frac{b^1{}_3\,\eta^1\,\eta^3}{b^3{}_3} + \frac{b^2{}_3\,\eta^2\,\eta^3}{b^3{}_3} - \eta^1\,\eta^1 - \eta^2\,\eta^2\right) \; .
$$

It can be an integer number in two particular cases : either $\eta^1 = \eta^2 = 0$ (hence $\eta^3 = \pm 1$), or at least one of the two components $b^1{}_3$ and $b^2{}_3$ is equal to zero. In the first case, we obtain :

$$
B^{-1}\Psi\,B = \begin{pmatrix} -\dfrac{b^1{}_2}{b^2{}_2} & -\dfrac{b^1{}_2\,b^1{}_2}{b^1{}_1\,b^2{}_2} - \dfrac{b^2{}_2}{b^1{}_1} & 0 \\[6pt] \dfrac{b^1{}_1}{b^2{}_2} & \dfrac{b^1{}_2}{b^2{}_2} & 0 \\[6pt] 0 & 0 & 0 \end{pmatrix} ,
$$

$$
B^{-1}\Psi^2\,B = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix} .
$$

Since $B^{-1}\Psi^2\,B$ contains only integer numbers, we need to consider only $B^{-1}\Psi\,B$. Multiplying it by $\sin\frac{\pi}{3} = \frac{\sqrt{3}}{2}$, we see that the 2×2 block containing the components different

from zero is almost the same as the $B^{-1}FB$ matrix obtained in two dimensions (in the case of $\alpha = \frac{\pi}{3}$). Following the same argument, we find :

$$
B = \begin{pmatrix} 1 & \frac{1}{2} & 0 \\ 0 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} , \quad B = \begin{pmatrix} 1 & -\frac{1}{2} & 0 \\ 0 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} .
$$

According to the first remark on page 113, there is an infinity of other possible matrices, obtained by adding any integer number to the component $(1; 2)$ of one of the matrices right above. In the case where $\eta^1 \neq 0$ or $\eta^2 \neq 0$, or both, then $b^1{}_3 \neq 0$, or $b^2{}_3 \neq 0$ or both. One solution is obtained when considering two of the three upper non-diagonal components equal to zero. We then obtain analogous matrices as those obtained above :

$$
\begin{pmatrix} 1 & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix} , \quad \begin{pmatrix} 1 & 0 & -\frac{1}{2} \\ 0 & 1 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix} ,
$$

and :

$$
\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \frac{1}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix} , \quad \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & -\frac{1}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix} .
$$

All these matrices correspond to the transformation of one of the canonical basis vectors which has been under the effect of a rotation of angle $\pm\frac{\pi}{6}$ around the subspace spanned by one of the two other vectors of the basis. In the two-dimensional case, we observe the same, the only minor difference being that the rotation is around a subspace of dimension zero (and not one). In the three-dimensional case, a lattice $\Lambda = \{B\lambda \mid \lambda \in \mathbb{Z}^3\}$, where B is one of the six matrices derived above, is called *trigonal* or *hexagonal*. Note that these matrices are not the only possible ones; rotations of angle $\frac{\pi}{3}$ can also be obtained in the case where all the diagonal and upper-diagonal elements of B are different from zero. In any event, such a situation can be reduced to one of the cases treated above, by considering a change of basis and applying a rotation; this will be explained below.

If we calculate the explicit form of $B^{-1}\exp(\alpha\,\Psi)\,B$, where B is one of the six matrices obtained just above, and follow the same method as in the case of the cubic lattice for finding all the possible values of α for which $B^{-1}\exp(\alpha\,\Psi)\,B$ has only integer number, we notice that α is never equal to $\frac{\pi}{2}$ and $\frac{3\pi}{2}$. This implies that the set $O_3(\mathbb{Z})$, that is the set of all matrices transforming a cubic lattice to itself, is not a subgroup of all matrices F transforming $\Lambda = \{B\lambda \mid \lambda \in \mathbb{Z}^3\}$ into itself. In conclusion, none of these two sets is a subgroup of the other.

This fact can also be shown in a less formal way, by considering any vector and rotation of angle $\frac{2\pi}{N}$, where $N \in \{1; 2; 3; 4; 6\}$. Without loss of generality, we consider a rotation around an axis, a subspace of dimension one spanned by the vector $e_3 = (0; 0; 1)$ of the canonical basis $\{e_1; e_2; e_3\}$ of $\mathbb{R}^3$ and any vector v forming an angle $\theta \in [0; \frac{\pi}{2}[$, where $m \in \mathbb{Z}$, with e_3, the expression of which with respect to the canonical basis is $v = (v^1; v^2; v^3)$.

- $N = 1$. Any vector v is transformed into itself. Any three independent vectors generate a three-dimensional finite free $\mathbb{Z}$-module which is left invariant under a rotation of angle 0. These three vectors can, in particular, form an orthonormal basis, generating a cubic lattice.

- $N = 2$. From v, a rotation of angle π generates a vector $v' = (-v^1; -v^2; v^3)$ which is linearly independent of v (as the angle between v and e_3 is different from πm, $m \in \mathbb{Z}$). These two vectors generate a two-dimensional $\mathbb{Z}$-module in the plane spanned by them. To obtain a three-dimensional $\mathbb{Z}$-module, we need a third vector $w = (w^1; w^2; w^3)$ independent of v and v', that is outside the plane spanned by v and v'. The image of w through the rotation of angle π is $w' = (-w^1; -w^2; w^3)$. We have four vectors v, v', w and w' which cannot be linearly independent in a three-dimensional vector space. Let us choose three of them, for instance v, v' and w, and consider them as a basis of a three-dimensional finite free $\mathbb{Z}$-module. If this module is transformed into itself through the rotation of angle π, then w' must be an element of it, that is $w' = a\,v + b\,v' + c\,w$, with $a, b, c \in \mathbb{Z}$. We immediately see that a solution is obtained if $a = b = 1$ and $c = -1$, hence $w^3 = 2\,v^3 - w^3 \Leftrightarrow w^3 = v^3$. We conclude that the three vectors $v = (v^1; v^2; v^3)$, $v' = (-v^1; -v^2; v^3)$ and $w = (w^1; w^2; v^3)$ (where $v^1, v^2, v^3, w^1, w^2 \in \mathbb{R}$, $v^3 \neq 0$), such that w is not in the same plane as v and v', form a basis of a $\mathbb{Z}$-module which is transformed into itself through a rotation of angle π around the subspace spanned by e_3. From these vectors and their images through the rotation, we can obtain other sets of three vectors, for instance $v + v' = (0; 0; 2\,v^3)$, $v - v' = (2\,v^1; 2\,v^2; 0)$ and $w - w' = (2\,w^1; 2\,w^2; 0)$, or just v, v' and $w - w'$. All these vectors, as well as their images through the rotation of angle π, are elements of the $\mathbb{Z}$-module spanned by v, v' and w. If $v^1 = v^3 = w^2 = \frac{1}{2}$ and $v^2 = w^1 = 0$, then $v + v'$, $v - v'$ and $w - w'$ form an orthonormal basis; it spans a cubic lattice and the rotation of angle π corresponds to that around a main direction in a cube. If $v^1 = v^3 = \frac{1}{\sqrt{2}}$, $w^2 = 1$ and $v^2 = w^1 = 0$, then v, v' and $w - w'$ constitute an orthonormal basis; it also spans a cubic lattice and the rotation of angle π is that around any face diagonal.

- $N = 3$. Successive applications of a rotation of angle $\frac{2\pi}{3}$ to $v = (v^1; v^2; v^3)$ generate the vectors $v' = \left(-\frac{v^1 + \sqrt{3}\,v^2}{2}; \frac{\sqrt{3}\,v^1 - v^2}{2}; v^3\right)$ and $v'' = \left(\frac{-v^1 + \sqrt{3}\,v^2}{2}; -\frac{\sqrt{3}\,v^1 + v^2}{2}; v^3\right)$. These three vectors form a basis and generate a three-dimensional $\mathbb{Z}$-module. If we consider $v^1 = v^2 = v^3 = 1$, then v, v' and v'' form an orthonormal basis; it spans a cubic lattice and the rotation of angle $\frac{2\pi}{3}$ corresponds to that around any space diagonal in a cube. Note that $v - v''$, $v' - v$ and $v + v' + v''$ form a basis generating a $\mathbb{Z}$-module which is also transformed into itself through the same rotation of angle $\frac{2\pi}{3}$.

- $N = 4$. If we apply successive rotations of angle $\frac{\pi}{2}$ to the vector $v = (v^1; v^2; v^3)$, we obtain the three vectors $v' = (-v^2; v^1; v^3)$, $v'' = (-v^1; -v^2; v^3)$ and $v''' = (v^2; -v^1; v^3)$. Any three of these four vectors form a basis and the fourth can be written as a linear combination of the other three, with only integer coeffi-

cients. Let us consider for instance v, v' and v''. These three vectors span a three-dimensional finite free $\mathbb{Z}$-module which is transformed into itself through a rotation of angle $\frac{\pi}{2}$ around the subspace generated by e_3. The v''' is an element of this module which is written as $v''' = v - v' + v''$. From v, v' and v'' and v''', we can obtain other sets of vectors, for instance $v - v''$, $v' - v'''$ and $v + v''$ ($= v' + v'''$). All these vectors, as well as their images through the rotation of angle $\frac{\pi}{2}$, are elements of the $\mathbb{Z}$-module spanned by v, v' and v''. If $v^1 = v^2 = v^3 = \frac{1}{2}$, then $v - v''$, $v' - v'''$ and $v + v''$ constitute an orthonormal basis; it spans a cubic lattice and the rotation of angle $\frac{\pi}{2}$ correspond to that around any main direction in a cube.

- $N = 6$. Successive applications of a rotation of angle $\frac{\pi}{3}$ to the vector v generate five other vectors v', v'', v''', v^{iv} and v^{v}, the tip of which form, with that of v, a regular hexagon. Any integer combination of these six vectors forms a $\mathbb{Z}$-module which is transformed into itself through a rotation of angle $\frac{\pi}{3}$. To obtain a basis of this module, we cannot choose any three vectors among the six above. For instance, v, v' and v'' constitute a basis of this module, whereas v, v'' and v^{iv} do not. In any event, a basis of such a module can never be orthonormal. The set of vectors $v - v^{\text{iv}}$, $v'' - v$ and $v + v'' + v^{\text{iv}}$ constitutes a basis which generates a three-dimensional finite free $\mathbb{Z}$-module such that the rotation of angle $\frac{\pi}{3}$ transforms it into itself. This basis is indeed the same as the one obtained for $N = 3$. However, the vectors v, v'' and v^{iv} generate a module being left invariant only under rotations of angle $\frac{2\pi}{3}$ and not under those of angle $\frac{\pi}{3}$. This fact constitutes the main distinction between modules obtained in this case and those obtained in the case $N = 3$.

We conclude that any rotation of angle $\frac{2\pi}{N}$, with $N \leqslant 4$, transforming a three-dimensional finite free $\mathbb{Z}$-module into itself, corresponds to a rotation present in a cubic lattice. This implies that the set of matrices F transforming a three-dimensional (finite free) $\mathbb{Z}$-module into itself is a subgroup of $\mathrm{O}_3(\mathbb{Z})$ if and only if the considered module does not contain rotations of angle $\frac{\pi}{3}$. Thus, for any lattice $\Lambda = \{B\,\lambda \mid \lambda \in \mathbb{Z}^3\}$, where B is an invertible upper-triangular matrix, we first analyse if it is left invariant under rotations of angle $\frac{\pi}{3}$ (and multiples). If it is the case, Λ contains only rotations of angle $\frac{\pi}{3}$ and its multiples, in particular π. If not, Λ contains rotations which are all present in the cubic lattice. Thus, we take all the matrices $F \in \mathrm{SO}_n(\mathbb{Z})$, that is the matrices $F \in \mathrm{O}_n(\mathbb{Z})$ the determinant of which is $+1$, and calculate $[F; B]$. The subset of matrices F such that $[F; B] = 0_3$ corresponds to the group of rotations transforming Λ, seen as a $\mathbb{Z}$-module, into itself. Finally, the matrices F with determinant equal to -1 are obtained in the same way as for cubic lattice, based on the argument that the composition of a matrix of determinant -1 with itself corresponds to a rotation matrix.

With these considerations, all possible lattice systems in three dimensions may be deduced. As their shape is dictated by the rotation under which they are left invariant, they can be classified according to the angle of rotation. To each system, a general form of the matrix B is given.

- $N = 1$. The matrix B is any upper-triangular matrix with positive determinant. The corresponding lattice is called *triclinic*.

- $N = 2$. We have :

$$B = \begin{pmatrix} b^1_1 & b^1_2 & 0 \\ 0 & b^2_2 & 0 \\ 0 & 0 & b^3_3 \end{pmatrix}, \quad B = \begin{pmatrix} b^1_1 & 0 & b^1_3 \\ 0 & b^2_2 & 0 \\ 0 & 0 & b^3_3 \end{pmatrix} \quad \text{or} \quad B = \begin{pmatrix} b^1_1 & 0 & 0 \\ 0 & b^2_2 & b^2_3 \\ 0 & 0 & b^3_3 \end{pmatrix},$$

  where the diagonal elements can be considered to be strictly positive. These three matrices are equivalent, in the sense that the shape of the module generated by the three vectors $B\,e_1$, $B\,e_2$ and $B\,e_3$, where $\{e_1; e_2; e_3\}$ is the canonical basis), is similar : one of the basis vector is always perpendicular to each of the two others. The generated lattice is called *monoclinic*. Traditionally, the second matrix above is used; the rotation of angle π is around e_2. In the special case where

$$B = \begin{pmatrix} b^1_1 & 0 & 0 \\ 0 & b^2_2 & 0 \\ 0 & 0 & b^3_3 \end{pmatrix},$$

  the lattice is called *orthorhombic*. The three vectors $B\,e_1$, $B\,e_2$ and $B\,e_3$ are orthogonal and the generated $\mathbb{Z}$-module is left invariant under rotations of angle π around each of these three vectors.

- $N = 3$. Then :

$$B = b \begin{pmatrix} 1 & \pm\frac{1}{2} & 0 \\ 0 & \frac{\sqrt{3}}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad B = b \begin{pmatrix} 1 & 0 & \pm\frac{1}{2} \\ 0 & 1 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix} \quad \text{or} \quad B = b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \pm\frac{1}{2} \\ 0 & 0 & \frac{\sqrt{3}}{2} \end{pmatrix},$$

  where $b \in \mathbb{R}^*_+$. To all of these three matrices corresponds a same kind of lattice, called *trigonal*; among the three vectors $B\,e_1$, $B\,e_2$ and $B\,e_3$, one is perpendicular to the two others and the angle between the two others is equal to $\frac{\pi}{3}$ or $\frac{2\pi}{3}$. Traditionally, the first matrix, with a positive non-diagonal element is considered. Thus, the rotation axis is the one-dimensional subspace spanned by e_3. Another kind of basis is obtained by taking $B\,(e_1 + e_3)$, $B\,(-e_1 + e_2 + e_3)$ and $B\,(-e_2 + e_3)$. The corresponding lattice is called *rhombohedral*.

- $N = 4$. Then :

$$B = \begin{pmatrix} b^1_1 & 0 & 0 \\ 0 & b^1_1 & 0 \\ 0 & 0 & b^3_3 \end{pmatrix}, \quad B = \begin{pmatrix} b^1_1 & 0 & 0 \\ 0 & b^2_2 & 0 \\ 0 & 0 & b^2_2 \end{pmatrix} \quad \text{or} \quad B = \begin{pmatrix} b^3_3 & 0 & 0 \\ 0 & b^2_2 & 0 \\ 0 & 0 & b^3_3 \end{pmatrix}.$$

  The corresponding lattice is called *tetragonal*. Traditionally, the first matrix is considered; thus, the rotation axis is around e_3.

- The *cubic* lattice corresponds to the case where $B = I_3$ or $B = a\,I_3$, with $a \in \mathbb{R}^*_+$. Its shape is a particular case of the three previous and contains all the rotations existing there.

- $N = 6$. The matrices B are the same as for $N = 3$. The corresponding lattice, which is left invariant under rotations of angle $\frac{\pi}{3}$, is called *hexagonal*.

As seen in the remarks written in the beginning of this subsection, the shape of B is not unique; for a same group $\{F \in O_3(\mathbb{R}) \mid B^{-1}F B \in GL_3(\mathbb{R})\}$, different matrices B can be found.

n-dimensional lattices $(n > 3)$:
Any matrix $F \in SO_n(\mathbb{R})$, with $n > 3$, is orthogonally similar to an orthogonal matrix $\bar{F}$ containing more than one 2×2 block

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

in the diagonal. This implies that the cosinus of more than one angle appears in the trace of $\bar{F}$. Thus, to find all possible angles of rotation transforming an n-dimensional lattice into itself, we cannot use the fact that the trace of the matrix must be an integer number. It becomes then difficult to classify the matrices B (characterising a lattice) into lattice systems. The best way to obtain all possible rotations is probably to explicitly calculate $B^{-1} \exp(\alpha\, \Psi)\, B$, where $\Psi \in \mathfrak{o}_n(\mathbb{R})$ and $\alpha \in \mathbb{R}$, for many different B, and find the values of α and the matrix Ψ such that $B^{-1} \exp(\alpha\, \Psi)\, B \in GL_n(\mathbb{Z})$. The decomposition of an orthogonal matrix according to theorem 4.1.1 can be used as an alternative form for $\exp(\alpha\, \Psi)$. In any event, note that for each lattice characterised by the matrix B, at least a part of the matrices F such that $B^{-1}F B \in GL_n(\mathbb{Z})$ can be obtained just by taking all $F \in O_n(\mathbb{Z})$, that is all F transforming a n-dimensional cubic lattice into itself, which commute with B. However, the difficulty consists in finding if there are other matrices F which do not belong to $O_n(\mathbb{R})$. For that, a computer might be useful...

In conclusion, the Lie group formalism offers a good framework for methodically studying the matrix part of symmetry operations of any lattice, at least in the case of low-dimensional spaces. In the case of a cubic lattice, all the matrices F transforming it into itself have been obtained; in the three-dimensional case, it provides a proof that rotations of angle $\frac{\pi}{3}$ do not exist in the cubic lattice, while they exist in certain other three-dimensional lattices. Note that this result can be alternatively obtained by considering tilings of the two-dimensional sphere in the three-dimensional Euclidean space (more information can be for instance obtained in the textbook [SC06]). In higher dimensional cases, corollary 4.1.4 offers an easier alternative for finding all matrices $F \in O_n(\mathbb{Z})$. Thanks to the one-parameter subgroups, the lattice systems can easily be treated and classified, especially in two and three dimensions. A direct connection between the shape of a lattice and the angle of rotation under which it is left invariant can be established methodically. A more detailed classification, based on general features of a vector basis, like right angles or equal length of basis vectors, might be envisaged; it would imply the definition of several additional equivalence relations between the matrices characterising the shape of a lattice.

It has been shown that the matrix part of any symmetry operation of a given lattice $\Lambda = \{B\, \lambda \mid \lambda \in \mathbb{Z}^n\}$ (expressed with respect to a natural coordinate system) must

belong to the set $\{F \in \mathrm{O}_3(\mathbb{R}) \mid B^{-1}FB \in \mathrm{GL}_3(\mathbb{Z})\}$ and its translation part must be an element of Λ. In the case of a real crystal structure in the Euclidean manifold, with which the lattice Λ is associated, the set of the matrix parts of all of its symmetry operations is not necessarily equal to the group $\{F \in \mathrm{O}_3(\mathbb{R}) \mid B^{-1}FB \in \mathrm{GL}_3(\mathbb{Z})\}$, it may be just a subgroup. For any symmetry operation ϕ of a crystal structure, the matrix part of which is F, there exists an $N \in \mathbb{N} \smallsetminus \{0\}$ such that $F^N = I_n$. The condition that the translation part of ϕ must satisfy is that N compositions of ϕ correspond to an element of the lattice Λ associated to the crystal. From then on, all the possible three-dimensional space group operations may be directly derived.

Chapter 5

Diffraction Pattern of a Structure

Diffraction by X-rays, neutrons or electrons constitutes a powerful tool for studying crystals at the atomic scale. The ideal diffraction patterns are characterised by a countable set of spots with different intensities. X-rays interact with the electron density of the atoms, while neutrons mostly interact with the nucleus; electron beams are sensitive to the electrostatic potential created by the nucleus and electron densities of each atom. In all three cases, the diffraction is considered *elastic*, *i.e.* the incident and diffracted beams have the same wavelength. Inelastic scattering also exists, but its effects are of lesser importance (except in the case of electron beams) and considered as parasite rays in the measurements; it will therefore be neglected.

In this chapter, we shall focus on X-ray diffraction. The appropriate mathematical tool for describing this phenomenon is the Fourier transform. Indeed, it turns out that the square of the modulus of the Fourier transform of the electron density of a crystal is proportional to the intensity of the diffracted beams [SC06]. Using the results obtained in the previous chapters, we shall show that the electron density of a crystal in a manifold (*i.e.* whether modulated or not), can be obtained by applying to the electron density of one unit cell the exponential of a finite free $\mathbb{Z}$-module of the Lie algebra associated with the translation group of the considered manifold. This will illustrate that an electron density, as well as its Fourier transform, can be split into two parts, the first one in which appears the geometry of the space in which the crystal exists, and the other which contains the elements of the translation group. The geometry of a space, *i.e.* the parameterisation of this latter, and the translation group are two different objects which, when *blended* together, generate pictures like those obtained from diffraction.

5.1   Fourier Transform of the Electron Density

The appropriate framework for studying the Fourier transform is the Schwartz space $\mathcal{SCH}(\mathbb{R}^n)$ (see appendix C), as this space is closed under the Fourier transform operation : the Fourier transform of any function of $\mathcal{SCH}(\mathbb{R}^n)$ is also a function of $\mathcal{SCH}(\mathbb{R}^n)$. However, for crystallographic applications, other functions, which are not in $\mathcal{SCH}(\mathbb{R}^n)$ must be taken into account. Thanks to the theory of distributions, such functions can be treated in the frame of the Schwartz space as well, without creating any problem.

5.1.1 Structure in the Manifold

For an n-dimensional crystal structure, one assumes that the electron density ρ of an atom α is described by a function of $\mathcal{SCH}(\mathbb{R}^n)$, which can be written as :

$$
\begin{aligned}
\mathbb{R}^n &\longrightarrow \mathcal{SCH}(\mathbb{R}^n) \\
r &\longmapsto \rho_\alpha(r - r_\alpha) \, ,
\end{aligned}
$$

where $r = (r^1; \ldots; r^n)$ is an n-dimensional variable and $r_\alpha = (r_\alpha{}^1; \ldots; r_\alpha{}^n)$ are the coordinates of the centre of the considered atom in $\mathbb{R}^n$. These coordinates correspond to the natural coordinates of the n-dimensional Euclidean manifold $\mathbb{R}^n$. The reason for using here r instead of u will become clear further on. The shape of ρ depends on the kind of atom; the function reaches its maximum values in a neighbourhood of the centre of the atom and it vanishes when the norm of $r - r_\alpha$ tends to infinity.

In chapter 2, we have seen that modulated structures are described in a manifold M which corresponds to $\mathbb{R}^n$, parameterised by the one-to-one map $H : \mathbb{R}^n \to M \cong \mathbb{R}^n$ which is the sum of the identity map and a wave function of the position. This function H carries the position u of an atom in the average structure in $\mathbb{R}^n$ to the displaced position $r = H(u) \in \mathbb{R}^n$. A different letter is used for the same natural coordinate system in $\mathbb{R}^n$, in order to distinguish the domain and the target; to be precise, we have $r^j = u^j \circ H(u) = h^j(u)$, where $H = (h^1; \ldots; h^n)$. Electron densities on M are therefore elements of $\mathcal{SCH}(\mathbb{R}^n)$.

Let us consider $r_\alpha = H(u_\alpha)$. Then, the function $r \mapsto \rho_\alpha\big(r - H(u_\alpha)\big)$ is the electron density of an atom α centred at the point of coordinates $H(u_\alpha)$. It can be written as :

$$
r \longmapsto \rho_\alpha(r - H(u_\alpha + u))\big|_{u=0} \, . \tag{5.1.1}
$$

Let $\sum_{j=1}^n (B\,\lambda)^j\, W_j$ be an element of $\mathfrak{Z}_B^n \subset \mathfrak{trans}(M)$ (see corollary 2.2.13), where $W_j = I_n\, \partial_j$, with $\partial_j = \frac{\partial}{\partial u^j}$, and B the matrix characterising the geometry of the lattice associated with the average structure of the modulated crystal to which the atom α belongs. Then :

$$
\exp\left(\sum_{j=1}^n (B\,\lambda)^j\, W_j\right) \rho_\alpha\big(r - H(u_\alpha + u)\big)\Big|_{u=0} = \rho_\alpha\big(r - H(u_\alpha + B\,\lambda)\big) \tag{5.1.2}
$$

Indeed, ρ_α can be considered as a function of $u = (u^1; \ldots; u^n)$:

$$
\rho_\alpha\big(r - H(u_\alpha + u)\big) = \tilde\rho_\alpha(u) \, ;
$$

thus :

$$
\exp\left(\sum_{j=1}^n (B\,\lambda)^j\, W_j\right) \tilde\rho_\alpha(u^1; \ldots; u^n) = \tilde\rho_\alpha(u) + \sum_{l=1}^n (B\,\lambda)^j\, \frac{\partial\tilde\rho_\alpha(u)}{\partial u^j} +
$$

$$
+ \frac{1}{2} \sum_{j_1, j_2=1}^n (B\,\lambda)^{j_1} (B\,\lambda)^{j_2}\, \frac{\partial^2\tilde\rho_\alpha(u)}{\partial u^{j_1}\, \partial u^{j_2}} + \ldots
$$

$$
+ \frac{1}{r!} \sum_{j_1, \ldots, j_r=1}^n (B\,\lambda)^{j_1} \cdots (B\,\lambda)^{j_r}\, \frac{\partial^r\tilde\rho_\alpha(u)}{\partial u^{j_1} \ldots \partial u^{j_r}} + \ldots
$$

which exactly corresponds to the Taylor series of $\tilde{\rho}$ about u. Summing expression 5.1.2 over $\lambda \in \mathbb{Z}^n$, we obtain the electron density of all the atoms α of the structure.

Let us consider the domain

$$\mathcal{D} = \{B\,\nu \mid \nu = (\nu^1;\,\ldots;\,\nu^n),\ 0 \leqslant \nu^i < 1,\ \forall\ 1 \leqslant i \leqslant n\} \ .$$

$\mathcal{D}$ is called the *(primitive) unit cell* of the average structure and, by analogy, $\tilde{\mathcal{D}} \doteq H(\mathcal{D})$ is the (primitive) unit cell of the corresponding modulated crystal. Suppose that μ atoms (some different, some similar) lie in $\mathcal{D}$ (in the average structure), the centres of which are at the positions u_α, $1 \leqslant \alpha \leqslant \mu$. Their positions in the modulated structure are $H(u_\alpha)$. The electron density of all these atoms is then :

$$\rho_{\text{cell}}(r) = \sum_{\alpha=1}^{\mu} \rho_\alpha\big(r - H(u_\alpha)\big) \ . \tag{5.1.3}$$

Let us write :

$$\rho_{\text{cell},u}(r) = \sum_{\alpha=1}^{\mu} \rho_\alpha\big(r - H(u_\alpha + u)\big) \ , \tag{5.1.4}$$

and consider ρ_{cell} as a function of u, too. Applying to this latter the exponential of an element $\sum_{j=1}^{n}(B\,\lambda)^j\,W_j$, taking its value at $u = 0$ and summing over $\lambda \in \mathbb{Z}^n$, we obtain the electron density $\rho(r)$ of the whole modulated structure :

$$
\begin{aligned}
\rho(r) \ &\doteq\ \left[\sum_{\lambda\in\mathbb{Z}^n} \exp\left(\sum_{j=1}^{n}(B\,\lambda)^j\,W_j\right) \rho_{\text{cell},u}(r) \right]_{u=0} = \\[2mm]
&=\ \left[\sum_{\lambda\in\mathbb{Z}^n} \exp\left(\sum_{j=1}^{n}(B\,\lambda)^j\,W_j\right) \sum_{\alpha=1}^{\mu} \rho_\alpha\big(r - H(u_\alpha + u)\big) \right]_{u=0} = \\[2mm]
&=\ \left[\sum_{\lambda\in\mathbb{Z}^n}\sum_{\alpha=1}^{\mu} \exp\left(\sum_{j=1}^{n}(B\,\lambda)^j\,W_j\right) \rho_\alpha\big(r - H(u_\alpha + u)\big) \right]_{u=0} = \\[2mm]
&=\ \sum_{\lambda\in\mathbb{Z}^n}\sum_{\alpha=1}^{\mu} \rho_\alpha\big(r - H(u_\alpha + B\,\lambda)\big) \ . \tag{5.1.5}
\end{aligned}
$$

In the case where $H = \text{id}$, we obtain the electron density of the average structure. As in chapter 2, we see again that from the electron density of a unit cell, the same set $\mathfrak{Z}_B^n$ generates the electron density of the whole structure, be it modulated or not.

In order to find the Fourier transform of ρ, we can either take the last expression of relation 5.1.5 and do a traditional calculation, or consider the first expression and exploit the fact that the variable r appears only in $\rho_{\text{cell},u}$. Following the second way, we

obtain :

$$
\begin{aligned}
(\mathcal{F}\rho)(k) &= \int_{\mathbb{R}^n} \left[\sum_{\lambda \in \mathbb{Z}^n} \exp\left(\sum_{j=1}^n (B\,\lambda)^j\, W_j \right) \rho_{\mathrm{cell},u}(r) \right]_{u=0} \exp(\mathrm{i}\,k \cdot r)\, \mathrm{d}^n r = \\[2ex]
&= \left[\sum_{\lambda \in \mathbb{Z}^n} \exp\left(\sum_{j=1}^n (B\,\lambda)^j\, W_j \right) \int_{\mathbb{R}^n} \rho_{\mathrm{cell},u}(r) \exp(\mathrm{i}\,k \cdot r)\, \mathrm{d}^n r \right]_{u=0} = \\[2ex]
&= \left[\sum_{\lambda \in \mathbb{Z}^n} \exp\left(\sum_{j=1}^n (B\,\lambda)^j\, W_j \right) \int_{\mathbb{R}^n} \sum_{\alpha=1}^\mu \rho_\alpha\big(r - H(u_\alpha + u)\big) \exp(\mathrm{i}\,k \cdot r)\, \mathrm{d}^n r \right]_{u=0} ,
\end{aligned}
$$

where $\cdot$ is the Euclidean scalar product, given by $k \cdot r = \sum_{a=1}^n k_a\, r^a$ (note that $k_a = \sum_{b=1}^n \delta_{ab}\, k^b = k^a$). Up to this point, there was no need to specify H further. In the following calculations, H shall be considered as the sum of the identity and a *displacement* function $\tilde{H}$, that is $H(u) = u + \tilde{H}(u)$. Thus :

$$
\rho_\alpha\big(r - H(u_\alpha + u)\big) = \rho_\alpha\big(r - u_\alpha - u - \tilde{H}(u_\alpha + u)\big) .
$$

Considering the change of variable $\tilde{r} = r - u - \tilde{H}(u_\alpha + u)$, we obtain :

$$
\begin{aligned}
(\mathcal{F}\rho)(k) &= \left[\sum_{\lambda \in \mathbb{Z}^n} \exp\left(\sum_{j=1}^n (B\,\lambda)^j\, W_j \right) \cdot \right. \\[2ex]
&\qquad \left. \cdot \int_{\mathbb{R}^n} \sum_{\alpha=1}^\mu \rho_\alpha(\tilde{r} - u_\alpha) \exp\big(\mathrm{i}\,k \cdot (\tilde{r} + u + \tilde{H}(u_\alpha + u))\big)\, \mathrm{d}^n \tilde{r} \right]_{u=0} = \\[2ex]
&= \left[\sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^\mu \exp\left(\sum_{j=1}^n (B\,\lambda)^j\, W_j \right) \exp\big(\mathrm{i}\,k \cdot (u + \tilde{H}(u_\alpha + u))\big) \cdot \right. \\[2ex]
&\qquad \left. \cdot \int_{\mathbb{R}^n} \rho_\alpha(\tilde{r} - u_\alpha) \exp(\mathrm{i}\,k \cdot \tilde{r})\, \mathrm{d}^n \tilde{r} \right]_{u=0} = \\[2ex]
&= \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^\mu \exp\big(\mathrm{i}\,k \cdot (B\,\lambda + \tilde{H}(u_\alpha + B\,\lambda))\big) \cdot \\[2ex]
&\qquad \cdot \int_{\mathbb{R}^n} \rho_\alpha(\tilde{r} - u_\alpha) \exp(\mathrm{i}\,k \cdot \tilde{r})\, \mathrm{d}^n \tilde{r} = \\[2ex]
&= \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^\mu \exp\big(\mathrm{i}\,k \cdot (B\,\lambda)\big) \exp\big(\mathrm{i}\,k \cdot \tilde{H}(u_\alpha + B\,\lambda)\big) \cdot \\[2ex]
&\qquad \cdot \int_{\mathbb{R}^n} \rho_\alpha(\tilde{r} - u_\alpha) \exp(\mathrm{i}\,k \cdot \tilde{r})\, \mathrm{d}^n \tilde{r} . \qquad (5.1.6)
\end{aligned}
$$

Note that in this derivation, the calculation of the integral is completely independent of the exponential of elements of $\mathfrak{Z}_B^n$. Let us now suppose that $\tilde{H}$ is a periodic wave

function of the position, that is :

$$u \longmapsto \tilde{H}(u) = \tilde{H}(\xi \cdot u) ,$$

with $\tilde{H}(\xi \cdot u + \bar{T}) = \tilde{H}(\xi \cdot u)$, for a $\bar{T} \in \mathbb{R}_+^*$; note that this relation means that $\tilde{h}^j(\xi \cdot u + \bar{T}) = \tilde{h}^j(\xi \cdot u)$, for each $1 \leqslant j \leqslant n$, where $\tilde{H} = (\tilde{h}^1; \ldots; \tilde{h}^n)$. ξ is an element of $\mathbb{R}^n$ called wave vector of the wave function $\tilde{H}$. Let $U \in \mathrm{SO}_n(\mathbb{R})$ be a matrix such that all components of the column-vector $\xi' = U\,\xi$ are equal to zero, except the first one, the value of which is $\xi'^1 = \|\xi\| = \sqrt{\xi \cdot \xi}$. The same matrix U applied to the column-vector u defines $u' = U\,u$. Thus :

$$\xi \cdot u = {}^{\mathrm{t}}\xi\, u = {}^{\mathrm{t}}\xi'\, {}^{\mathrm{t}}U\, U\, u' = {}^{\mathrm{t}}\xi'\, u' = \|\xi\|\, u'^1 ,$$

and $\tilde{H}$ can be seen as a function of u'^1. Since it is periodic, there exists a $T \in \mathbb{R}_+^*$ such that

$$\tilde{H}(u'^1 + T) = \tilde{H}\big(\|\xi\|(u'^1 + T)\big) = \tilde{H}(\|\xi\|\, u'^1) , \quad \text{with} \quad T = \frac{\bar{T}}{\|\xi\|} ,$$

and $u'^1 \mapsto \exp\big(\mathrm{i}\,k \cdot \tilde{H}(u'^1)\big)$ is also a periodic function, with the same period T; indeed :

$$\exp\big(\mathrm{i}\,k \cdot \tilde{H}(u'^1 + T)\big) = \exp\left(\mathrm{i}\sum_{j=1}^n k_j\, \tilde{h}^j(u'^1 + T)\right) = \exp\left(\mathrm{i}\sum_{j=1}^n k_j\, \tilde{h}^j(u'^1)\right) =$$

$$= \exp\big(\mathrm{i}\,k \cdot \tilde{H}(u'^1)\big) .$$

It can then be developed into a Fourier series :

$$\exp\big(\mathrm{i}\,k \cdot \tilde{H}(u'^1)\big) = \sum_{m \in \mathbb{Z}} c_m(k;\, \xi)\, \exp(\mathrm{i}\,m\,\omega\,u'^1) , \qquad \text{with} \quad \omega = \frac{2\,\pi}{T} ,$$

where :

$$c_m(k;\, \xi) = \frac{1}{T} \int_t^{t+T} \exp\big(\mathrm{i}\,k \cdot \tilde{H}(u'^1)\big) \exp(-\mathrm{i}\,m\,\omega\,u'^1)\, \mathrm{d}u'^1 =$$

$$= \frac{1}{T} \int_t^{t+T} \exp\big(\mathrm{i}\,k \cdot \tilde{H}(u'^1) - \mathrm{i}\,m\,\omega\,u'^1\big)\, \mathrm{d}u'^1 .$$

The expression $\omega\,u'^1$ can be written :

$$\omega\,u'^1 = \frac{2\,\pi}{T}\, u'^1 = \frac{2\,\pi}{T\,\xi_1'}\, \xi_1'\, u'^1 = \frac{2\,\pi}{T\,\|\xi'\|}\, \xi' \cdot u' = \frac{2\,\pi}{T\,\|\xi\|}\, \xi \cdot u .$$

We can consider $T\,\|\xi\| = 1$. Indeed, even if it were not the case, we could define the vector $\bar{\xi} = \frac{\xi}{T\,\|\xi\|}$ and consider $\tilde{H}$ as a function of $\bar{\xi} \cdot u$. Thus :

$$\exp\big(\mathrm{i}\,k \cdot \tilde{H}(u'^1)\big) = \sum_{m \in \mathbb{Z}} c_m(k;\, \xi)\, \exp(2\,\pi\,\mathrm{i}\,m\,\xi \cdot u) .$$

Since $\exp\big(i\,k \cdot \tilde{H}(u'^1)\big) = \exp\big(i\,k \cdot \tilde{H}(\xi'_1\,u'^1)\big) = \exp\big(i\,k \cdot \tilde{H}(\xi \cdot u)\big)$, then :

$$\exp\big(i\,k \cdot \tilde{H}(\xi \cdot u)\big) = \sum_{m\in\mathbb{Z}} c_m(k;\,\xi)\exp(2\,\pi\,i\,m\,\xi \cdot u) \ ;$$

in particular :

$$\exp\Big(i\,k \cdot \tilde{H}\big(\xi \cdot (u_\alpha + B\,\lambda)\big)\Big) = \sum_{m\in\mathbb{Z}} c_m(k;\,\xi)\exp\big(2\,\pi\,i\,m\,\xi \cdot (u_\alpha + B\,\lambda)\big) \ .$$

The Fourier transform of ρ then becomes :

$$\begin{aligned}
(\mathcal{F}\rho)(k) \ &= \ \sum_{\lambda\in\mathbb{Z}^n}\sum_{\alpha=1}^{\mu}\exp\big(i\,k \cdot (B\,\lambda)\big)\sum_{m\in\mathbb{Z}} c_m(k;\,\xi)\exp\big(2\,\pi\,i\,m\,\xi \cdot (u_\alpha + B\,\lambda)\big)\ \cdot \\
&\qquad\qquad\qquad\qquad\qquad \cdot \int_{\mathbb{R}^n} \rho_\alpha(\tilde{r} - u_\alpha)\exp(i\,k\cdot\tilde{r})\,\mathrm{d}^n\tilde{r} \ = \\[2mm]
&= \ \sum_{\lambda\in\mathbb{Z}^n}\sum_{\alpha=1}^{\mu}\sum_{m\in\mathbb{Z}} c_m(k;\,\xi)\exp(2\,\pi\,i\,m\,\xi \cdot u_\alpha)\exp\big(i\,(k + 2\,\pi\,m\,\xi) \cdot (B\,\lambda)\big)\ \cdot \\
&\qquad\qquad\qquad\qquad\qquad \cdot \int_{\mathbb{R}^n} \rho_\alpha(\tilde{r} - u_\alpha)\exp(i\,k\cdot\tilde{r})\,\mathrm{d}^n\tilde{r} \ .
\end{aligned}$$

Considering the derivations done in example C.3.14 of appendix C, we finally obtain :

$$\begin{aligned}
(\mathcal{F}\rho)(k) = (2\,\pi)^n \det B^{-1} \sum_{m\in\mathbb{Z}} c_m(k;\,\xi) \sum_{\ell\in\mathbb{Z}^n} \delta\Big(k - 2\,\pi\big({}^{\mathrm{t}}(B^{-1})\,\ell - m\,\xi\big)\Big)\ \cdot \\
\cdot \sum_{\alpha=1}^{\mu} \int_{\mathbb{R}^n} \rho_\alpha(r - u_\alpha)\exp(i\,k\cdot r)\,\mathrm{d}^n r\ \exp(2\,\pi i\,m\,\xi \cdot u_\alpha)\,, \quad (5.1.7)
\end{aligned}$$

where δ is the n-dimensional *generalised Dirac function* (see appendix C). This formula shows that the Fourier transform of the electron density of a modulated structure is non-zero only when

$$k = 2\,\pi\big({}^{\mathrm{t}}(B^{-1})\,\ell - m\,\xi\big)\,, \quad \ell \in \mathbb{Z}^n,\ m \in \mathbb{Z}\,. \tag{5.1.8}$$

In the case where $H = \mathrm{id}$ (the identity map), all coefficients c_m are equal to zero, except $c_0 = 1$. Expression 5.1.7 becomes :

$$(\mathcal{F}\rho)(k) \ = \ (2\,\pi)^n \det B^{-1} \sum_{\ell\in\mathbb{Z}^n} \delta\big(k - 2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell\big) \sum_{\alpha=1}^{\mu} \int_{\mathbb{R}^n} \rho_\alpha(r - u_\alpha)\exp(i\,k\cdot r)\,\mathrm{d}^n r \ ;$$

$$\tag{5.1.9}$$

it is non-zero only when

$$k = 2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell\,, \quad \ell \in \mathbb{Z}^n\,. \tag{5.1.10}$$

5.1.1 Definition : Let :

$$\Lambda = \{B\,\lambda \mid \lambda \in \mathbb{Z}^n\}$$

be a lattice in the n-dimensional Euclidean space. Λ is called *direct lattice* and the set :

$$\Lambda^* = \{2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell \mid \ell \in \mathbb{Z}^n\}$$

is called *reciprocal lattice* of Λ.

5.1.2 Remark : In order to eliminate the factor $2\,\pi$ appearing in Λ^*, we introduce the variable $\bar{k} = \frac{k}{2\,\pi}$. Thus, we define the reciprocal lattice of Λ as :

$$\bar{\Lambda}^* = \{{}^{\mathrm{t}}(B^{-1})\,\ell \mid \ell \in \mathbb{Z}^n\}\ .$$

The lattice Λ, seen in the tangent space at the origin $\mathrm{T}_o\mathbb{R}^n$, has the structure of a $\mathbb{Z}$-module. A natural basis for Λ is $\{B\,e_1;\,\ldots;B\,e_n\}$, where $e_1,\,\ldots,e_n$ are the column-vectors constituting the canonical basis of $\mathbb{R}^n$ (the components of e_i are all equal to zero, except the i-th the value of which is 1); the vectors ${}^{\mathrm{t}}(B^{-1})\,e_1,\ldots,{}^{\mathrm{t}}(B^{-1})\,e_n$ form a basis of $\bar{\Lambda}^*$. Let us write $a_i = B\,e_i$ and $a_j^* = {}^{\mathrm{t}}(B^{-1})\,e_j$, for all $1 \leqslant i,j \leqslant n$; then :

$$a_i \cdot a_j^* = {}^{\mathrm{t}}a_i\,a_j^* = {}^{\mathrm{t}}e_i\,{}^{\mathrm{t}}B\,{}^{\mathrm{t}}(B^{-1})\,e_j = {}^{\mathrm{t}}e_i\,e_j = \delta_{ij} \tag{5.1.11a}$$

and

$$a_i^* \cdot a_j = {}^{\mathrm{t}}a_i^*\,a_j = {}^{\mathrm{t}}e_i\,B^{-1}B\,e_j = {}^{\mathrm{t}}e_i\,e_j = \delta_{ij}\ . \tag{5.1.11b}$$

These relations appear in a clearer way when considering the components of a_i and a_j^* :

$$a_i = \begin{pmatrix} b^1{}_i \\ \vdots \\ b^n{}_i \end{pmatrix} \qquad \text{and} \qquad a_j^* = \begin{pmatrix} \bar{b}^i{}_1 \\ \vdots \\ \bar{b}^j{}_n \end{pmatrix},$$

with $B = (b^i{}_j)^n_{i,j=1}$ and $B^{-1} = (\bar{b}^i{}_j)^n_{i,j=1}$. The sets $\{a_1;\,\ldots;\,a_n\}$ and $\{a_1^*;\,\ldots;\,a_n^*\}$ are both bases of $\mathrm{T}_o\mathbb{R}^n$ and are respectively called *direct basis* and *reciprocal basis*. Relations 5.1.11a and 5.1.11b are properties of these bases and express, in a way, the duality between the tangent space $\mathrm{T}_o\mathbb{R}^n$ and the cotangent space $\mathrm{T}_o^*\mathbb{R}^n$, that is the space of all differential maps $\mathrm{d}f$ of $f \in C_0^\infty(\mathbb{R}^n)$. This cotangent space is a vector space and its elements are called *one-forms*. If $(x^1;\,\ldots;\,x^n)$ is a coordinate system on a neighbourhood $\mathcal{U}$ of a manifold M, the one-forms $\mathrm{d}x^1,\ldots,\mathrm{d}x^n$ form a dual basis of the coordinate vector fields $\partial_1,\ldots,\partial_n$, where $\partial_i = \frac{\partial}{\partial x^i}$, $1 \leqslant i \leqslant n$, as $\mathrm{d}x^i(\partial_j) = \frac{\partial x^i}{\partial x^j} = \delta^i{}_j$ (where $\delta^i{}_j$ is the Kronecker symbol). Thus, in our case, if we write :

$$a_i = \sum_{l=1}^n b^l{}_i\,\partial_l \qquad \text{and} \qquad a^{\sharp j} = \sum_{m=1}^n \bar{b}^j{}_m\,\mathrm{d}u^m \tag{5.1.12}$$

with $\partial_l = \frac{\partial}{\partial u^l}$, we have :

$$\begin{aligned}
a^{\sharp i}(a_j) &= \sum_{m=1}^n \bar{b}^j{}_m\,\mathrm{d}u^m \left(\sum_{l=1}^n b^l{}_i\,\partial_l \right) = \sum_{l,m=1}^n \bar{b}^j{}_m\,b^l{}_i\,\mathrm{d}u^m(\partial_l) = \\
&= \sum_{l,m=1}^n \bar{b}^j{}_m\,b^l{}_i\,\delta^m{}_l = \sum_{l=1}^n \bar{b}^j{}_l\,b^l{}_i = \delta^i{}_j\ .
\end{aligned}$$

In particular, this relation holds when a_i, $1 \leqslant i \leqslant n$, and $a^{\sharp j}$, $1 \leqslant j \leqslant n$, are valued at the origin o. $(a^{\sharp 1}; \dots; a^{\sharp n})$ is the dual basis of $(a_1; \dots; a_n)$. The components of $a^{\sharp i}$ are equal to those of a_i^*, $1 \leqslant i \leqslant n$. This is the reason why, regrettably, the reciprocal basis is often referred to as the dual basis. In any case, we should keep in mind that the vectors $a_1^*, \dots, a_n^*$ valued at o belong to $T_o\mathbb{R}^n$ and not to $T_o^*\mathbb{R}^n$; this explains why their index is at the bottom and not at the top. In order to show that, under a basis change, it is transformed into the same way as the dual vectors $a^{\sharp i}$, $1 \leqslant i \leqslant n$, the index is also often written at the top, so that we have equivalent notations $a_i^* = a^{*i}$, $1 \leqslant i \leqslant n$. All these considerations show that the tangent and cotangent spaces at a point are isomorphic. The fact that a_i^* are elements of a tangent and not cotangent space causes a problem with units. Indeed, any vector a_i has a unit of distance, whereas a_i^* has a unit of inverse-distance. This problem disappear completely when the dual basis, instead of the reciprocal one, is considered. In this case, $\Lambda \in T_o\mathbb{R}^n$, $\bar{\Lambda}^* \in T_o^*\mathbb{R}^n$, and the Fourier transform should be defined as a map from $T_o\mathbb{R}^n$ to $T_o^*\mathbb{R}^n$. We shall return to this point in the next subsection.

5.1.3 Theorem : *Let ρ be the electron density of a crystal structure*

$$\tilde{\mathcal{S}} = \{ H(u_\alpha + B\,\lambda) \mid 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n \} \ ,$$

where $\Lambda = \{ B\,\lambda \mid \lambda \in \mathbb{Z}^n \}$ is the associated lattice of the corresponding average structure $\mathcal{S}$. Let also $\rho_{\mathrm{cell},u}|_{u=0}$ be the electron density of the atoms in one unit cell of $\tilde{\mathcal{S}}$ (see relation 5.1.4) and $\mathcal{F}\rho_{\mathrm{cell},u}|_{u=0}$ its Fourier transform. Then :

$$\rho(r) = \sum_{\lambda \in \mathbb{Z}^n} \exp\left(\sum_{j=1}^{n} (B\,\lambda)^j\, \partial_j \right) \rho_{\mathrm{cell},u}(r)\big|_{u=0}$$

and

$$(\mathcal{F}\rho)(k) = \sum_{\lambda \in \mathbb{Z}^n} \exp\left(\sum_{j=1}^{n} (B\,\lambda)^j\, \partial_j \right) (\mathcal{F}\rho_{\mathrm{cell},u})(k)\big|_{u=0} \ ;$$

the same module $\mathfrak{Z}_B^n \in \mathfrak{trans}(\mathbb{R}^n)$ (see corollary 2.2.13) generates ρ from ρ_{cell} and $\mathcal{F}\rho$ from $\mathcal{F}\rho_{\mathrm{cell}}$.

5.1.4 Remark : If we have a look at expressions 5.1.7 and 5.1.8, we see that $\mathcal{F}\rho$ is in particular non-zero when $k = 2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell$, that is on the node of the reciprocal lattice Λ^* of the lattice Λ associated with the average structure $\mathcal{S}$. Moreover, we notice that the part of expression 5.1.7 for which $m = 0$ is identical to relation 5.1.9. Thus, the Fourier transform of the electron density of a modulated structure has exactly the same values on the points $k = 2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell$ as that of the corresponding average structure. In a way, we can say that the Fourier transform straightens out the shape of a modulated structure; per contra, it generates additional points. Note that since $\mathcal{F}\rho$ is non-zero when $k = 2\,\pi\left({}^{\mathrm{t}}(B^{-1})\,\ell - \frac{m}{T\,\|\xi\|}\,\xi \right)$, so it is for $|\mathcal{F}\rho|^2$.

5.1.5 Definition : Let $\mathcal{F}\rho$ be the Fourier transform of the electron density ρ of a modulated structure. The points $k = 2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell$ are called *main reflections* and all the others for which $\mathcal{F}\rho \neq 0$ are called *satellite reflections*. The index m is called the *order* of the satellite reflection.

5.1.6 Remark : In the previous calculations, we have assumed that the electron density ρ_α of the atom α is the same in any modulated unit cell, only the position of the centre of the atom is different. The shape of ρ_α might however be different in each unit cell, as the modulation H distorts each cell of the crystal in a different way. Moreover, this shape may also be different from that in the average structure. Although these considerations are absolutely legitimate, the fact to take a unique ρ_α for all atoms α seems to be, according to proposition 5.1.10 in subsection 5.1.4, more than acceptable. Theorem 5.1.3 makes therefore sense.

5.1.2   Structure in the Tangent Space

Let us recall from chapter 2 that the representation $\tilde{\mathcal{T}}_o$ of a modulated structure $\tilde{\mathcal{S}}$ in the tangent space at the origin o is :

$$\tilde{\mathcal{T}}_o = \left\{ \Omega(0)\,(u_\alpha + B\,\lambda) \mid 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n \right\}\,,$$

where $\Omega = \left(\frac{\partial h^i}{\partial u^j}\right)^n_{i,j=1}$, $H = (h^1; \ldots; h^n)$. The corresponding electron density can be written as :

$$_{\mathrm{tg}}\rho(v) = \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha\big(v - \Omega(0)\,(u_\alpha + B\,\lambda)\big)\,. \tag{5.1.14}$$

In this expression, the electron density ρ_α of each atom α is considered to be the same as that in the case of the structure in the manifold, it is not turned according to the shape of $\Omega(0)\,\Lambda$. There is no physical reason for proceeding in such a way, as the structure in the tangent space does not describe reality and is rather a tool for coherent definitions of space and point group operations. The use of the same ρ_α is motivated by the wish to have a relatively simple way to connect the electron density of a crystal in the manifold and that in a tangent space (see subsection 5.1.3).

Geometrically speaking, the representation of a modulated structure in a tangent space has the shape of a non-modulated structure in the n-dimensional Euclidean manifold. This explains why $_{\mathrm{tg}}\rho$ can be written as a convolution product :

$$_{\mathrm{tg}}\rho = {}_{\mathrm{tg}}\rho_{\mathrm{cell}} * \delta_{\Omega(0)\Lambda}\,, \tag{5.1.15}$$

where :

$$_{\mathrm{tg}}\rho_{\mathrm{cell}}(v) = \sum_{\alpha=1}^{\mu} \rho_\alpha(v - \Omega(0)\,u_\alpha) \tag{5.1.16a}$$

and

$$\delta_{\Omega(0)\Lambda}(v) = \sum_{\lambda \in \mathbb{Z}^n} \delta(v - \Omega(0)\,\lambda)\,. \tag{5.1.16b}$$

The Fourier transform of $_{\text{tg}}\rho$ is then :

$$(\mathcal{F}_{\text{tg}}\rho)(\kappa) \;=\; (\mathcal{F}_{\text{tg}}\rho_{\text{cell}})(\kappa)\,(\mathcal{F}\delta_{\Omega(0)\,\Lambda})(\kappa) \;=\;$$

$$=\; \int_{\mathbb{R}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(v - \Omega(0)\,u_\alpha)\exp(\mathrm{i}\,\kappa\cdot v)\,\mathrm{d}^n v\,\cdot$$

$$\cdot \int_{\mathbb{R}^n} \sum_{\lambda\in\mathbb{Z}^n} \delta(\tilde{v} - \Omega(0)\,B\,\lambda)\exp(\mathrm{i}\,\kappa\cdot\tilde{v})\,\mathrm{d}^n\tilde{v} \;=\;$$

$$=\; \det(B^{-1}\,\Omega(0)^{-1}) \int_{\mathbb{R}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(v - \Omega(0)\,u_\alpha)\exp(\mathrm{i}\,\kappa\cdot v)\,\mathrm{d}^n v\,\cdot$$

$$\cdot \sum_{\ell\in\mathbb{Z}^n} \delta\bigl(\kappa - 2\,\pi\,{}^{\text{t}}(B^{-1}\Omega(0)^{-1})\,\ell\bigr)\;, \qquad (5.1.17)$$

where the result of example C.3.14 of appendix C has been used. This expression is non-zero only when :

$$\kappa = 2\,\pi\,{}^{\text{t}}(B^{-1}\,\Omega(0)^{-1})\,\ell\;, \quad \ell\in\mathbb{Z}^n\;, \qquad (5.1.18)$$

that is when :

$$\bar{\kappa} = {}^{\text{t}}(B^{-1}\,\Omega(0)^{-1})\,\ell\;, \quad \ell\in\mathbb{Z}^n\;, \qquad (5.1.19)$$

where $\bar{\kappa} = \frac{\kappa}{2\,\pi}$. Note that in the case where H is the identity map, then :

$$(\mathcal{F}_{\text{tg}}\rho)(\kappa) = \det B^{-1} \int_{\mathbb{R}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(v - u_\alpha)\exp(\mathrm{i}\,\kappa\cdot v)\,\mathrm{d}^n v \sum_{\ell\in\mathbb{Z}^n} \delta\bigl(\kappa - 2\,\pi\,{}^{\text{t}}(B^{-1})\,\ell\bigr)\;. \quad (5.1.20)$$

This expression is identical to expression 5.1.9, which is expected, since a crystal structure in the Euclidean manifold and its representation in the tangent space at the origin are exactly the same. $(\mathcal{F}_{\text{tg}}\rho)$ is non-zero only when :

$$\bar{\kappa} = {}^{\text{t}}(B^{-1})\,\ell\;, \quad \ell\in\mathbb{Z}^n\;. \qquad (5.1.21)$$

5.1.7 Definition : Let :

$$\Upsilon_o = \{\Omega(0)\,B\,\lambda \mid \lambda\in\mathbb{Z}^n\}$$

the representation of the lattice $\tilde{\Lambda} = \{H(B\,\lambda) \mid \lambda\in\mathbb{Z}^n\}$ in the tangent space T_oM (where M corresponds to $\mathbb{R}^n$, parameterised by H). The set :

$$\Upsilon_o^* = \{{}^{\text{t}}(B^{-1}\,\Omega(0)^{-1})\,\ell \mid \ell\in\mathbb{Z}^n\}$$

is called *reciprocal lattice* of Υ_o. Both lattices, Υ_o and Υ_o^*, have the structure of a $\mathbb{Z}$-module. Υ_o is called *direct lattice*.

5.1.8 Remark : The notions of direct and reciprocal lattices are in fact related to the concepts of direct and reciprocal bases. Natural bases for Υ_o and Υ_o^* are respectively $\{\Omega(0)\,B\,e_1;\,\ldots;\,\Omega(0)\,B\,e_n\}$ and $\{{}^{\text{t}}(B^{-1}\,\Omega(0)^{-1})\,e_1;\,\ldots;\,{}^{\text{t}}(B^{-1}\,\Omega(0)^{-1})\,e_n\}$, where $e_1,\ldots,e_n$ are the column-vectors forming the canonical basis of $\mathbb{R}^n$. With $\tilde{a}_i = \Omega(0)\,B\,e_i$,

$1 \leqslant i \leqslant n$, and $\tilde{a}_j^* = {}^{\mathrm{t}}(B^{-1}\,\Omega(0)^{-1})\,e_j$, $1 \leqslant j \leqslant n$, we immediately see that $\tilde{a}_i \cdot \tilde{a}_j^* = \tilde{a}_i^* \cdot \tilde{a}_j = \delta_{ij}$. This justifies the names of direct and reciprocal lattices given, respectively, to Υ_o and Υ_o^*. According to remark 5.1.2, it is more natural to consider Υ_o as a set in $\mathrm{T}_o M$ and Υ_o^* a set in $\mathrm{T}_o^* M$. Indeed, if we write :

$$a_i = \sum_{l=1}^{n} \tilde{b}_i^l\, \partial_l\big|_o \qquad \text{and} \qquad a^{\sharp j} = \sum_{m=1}^{n} \bar{\tilde{b}}_m^j\, \mathrm{d}u^m\big|_o \ ,$$

where $\Omega(0)\,B = \big(\tilde{b}_j^i\big)_{i,j=1}^n$ and $(\Omega(0)\,B)^{-1} = \big(\bar{\tilde{b}}_j^i\big)_{i,j=1}^n$, we obtain :

$$a^{\sharp i}(a_j) = \sum_{l,m=1}^{n} \bar{\tilde{b}}_m^j\, \tilde{b}_i^l\, \mathrm{d}u^m(\partial_l)\big|_o = \delta^i{}_j \ .$$

Thus, it appears that the more appropriate framework for the Fourier transform is the Schwartz space on the tangent and cotangent spaces at the origin o of the manifold M :

$$\mathcal{F} : \mathcal{SCH}(\mathrm{T}_o M) \ \longrightarrow \ \mathcal{SCH}(\mathrm{T}_o^* M)$$
$$\rho \ \longmapsto \ \mathcal{F}\rho \qquad .$$

Indeed, $\mathcal{F}$ has a friendly behaviour if the space in which the electron density is considered has the structure of a vector space. In the Euclidean case, any crystal structure in the manifold and its representation in the tangent space at the origin are completely identical, hence the Fourier transform of the electron density in the manifold and in the tangent space at the origin are completely the same. For modulated structures, this is however more complicated. The previous calculations would suggest considering the electron density of a structure in the tangent space and obtain its Fourier transform on the cotangent space at the origin; however, this result does not correspond to reality. It would make sense only if a connection between the Fourier transform of the electron density of the real structure and that of its tangent space representation could be established. This point will be treated in the next subsection. Note that the tangent and cotangent spaces both correspond to $\mathbb{R}^n$, the only difference lying in the base vectors and their units. The canonical basis vectors of $\mathbb{R}^n$ have no unit, while those of $\mathrm{T}_o M$ have a unit of distance and those of $\mathrm{T}_o^* M$ a unit of inverse-distance.

5.1.3   Connection between manifold and tangent space

In expression 5.1.14 for ${}_{\mathrm{tg}}\rho$, the argument, $\Omega(0)\,(u_\alpha + B\,\lambda)$ can be written in components as :

$$\sum_{j=1}^{n} \omega^i{}_j(0)\big(u_\alpha{}^j + (B\,\lambda)^j\big) = \sum_{j=1}^{n} \big(u_\alpha{}^j + (B\,\lambda)^j\big)\, \frac{\partial h^i(u)}{\partial u^j}\bigg|_{u=0} \ , \qquad (5.1.22)$$

where $\Omega = (\omega^i{}_j)_{i,j=1}^n = \big(\frac{\partial h^i}{\partial u^j}\big)_{i,j=1}^n$. To obtain $h^i(u_\alpha + B\,\lambda)$ from this expression, we need to apply the exponential of $\sum_{j=1}^{n}\big(u_\alpha{}^j + (B\,\lambda)^j\big)\,\partial_j$ to h^i and take the value of the resulting expression at $u = 0$. Since the exponential is given by its power series,

it appears, in the connection between $_{\mathrm{tg}}\rho$ and ρ, as an infinity of convolution products with Dirac functions. Indeed, let us first consider :

$$
r \longmapsto \delta\left(r - \frac{1}{2} \sum_{j_1,j_2=1}^{n} (u_\alpha + B\,\lambda)^{j_1} (u_\alpha + B\,\lambda)^{j_2} \frac{\partial^2 H(u)}{\partial u^{j_1} \partial u^{j_2}} \right) \ . \tag{5.1.23}
$$

The convolution of this function with $r \mapsto \rho_\alpha\big(r - \sum_{j=1}^{n}(u_\alpha + B\,\lambda)^j\, \partial_j H(u)\big)$ is

$$
\int_{\mathbb{R}^n} \rho_\alpha\left(r - r' - \sum_{j=1}^{n}(u_\alpha + B\,\lambda)^j\, \frac{H(u)}{\partial u^j} \right) \cdot
$$

$$
\cdot\, \delta\left(r' - \frac{1}{2} \sum_{j_1,j_2=1}^{n} (u_\alpha + B\,\lambda)^{j_1} (u_\alpha + B\,\lambda)^{j_2} \frac{\partial^2 H(u)}{\partial u^{j_1} \partial u^{j_2}} \right) \mathrm{d}^n r' \ ,
$$

that is

$$
\rho_\alpha\left(r - \sum_{j=1}^{n}(u_\alpha + B\,\lambda)^j\, \frac{\partial H(u)}{\partial u^j} - \frac{1}{2} \sum_{j_1,j_2=1}^{n} (u_\alpha + B\,\lambda)^{j_1} (u_\alpha + B\,\lambda)^{j_2} \frac{\partial^2 H(u)}{\partial u^{j_1} \partial u^{j_2}} \right) =
$$

$$
= \ \rho_\alpha\left(r - \Big(\sum_{j=1}^{n}(u_\alpha + B\,\lambda)^j\, \frac{\partial}{\partial u^j} + \frac{1}{2} \sum_{j_1,j_2=1}^{n} (u_\alpha + B\,\lambda)^{j_1} (u_\alpha + B\,\lambda)^{j_2} \frac{\partial^2}{\partial u^{j_1} \partial u^{j_2}} \Big) H(u) \right) \ ;
$$

the first and second terms of the Taylor series of H appear in the argument of ρ_α. Taking this function and calculating the convolution product with

$$
r \longmapsto \delta\left(r - \frac{1}{3!} \sum_{j_1,j_2,j_3=1}^{n} (u_\alpha + B\,\lambda)^{j_1} (u_\alpha + B\,\lambda)^{j_2} (u_\alpha + B\,\lambda)^{j_3} \frac{\partial^3 H(u)}{\partial u^{j_1} \partial u^{j_2} \partial u^{j_3}} \right) \ ,
$$
$$\tag{5.1.24}$$

we obtain a function ρ_α in the argument of which the first, second and third terms of the Taylor series appear. Continuing this procedure, we finally obtain a function ρ_α such that all the terms of the Taylor series of H (the zeroth term, if it is not equal to zero, also needs to be considered) appear in its argument. Let :

$$
_{\mathrm{tg}}\rho_\alpha(r) \doteq \rho_{\alpha,u}\left(r - \sum_{j=1}^{n}(u_\alpha + B\,\lambda)^j\, \partial_j H(u) \right) \tag{5.1.25}
$$

and :

$$
\delta_{\mathrm{D}_{\alpha,\lambda}^m H(u)}(r) \doteq \delta\left(r - \frac{1}{m!} \sum_{j_1,\dots,j_m=1}^{n} (u_\alpha + B\,\lambda)^{j_1} \dots (u_\alpha + B\,\lambda)^{j_m} \frac{\partial^m H(u)}{\partial u^{j_1} \dots \partial u^{j_m}} \right) \ ,
$$
$$\tag{5.1.26}$$

where the variable v has been replaced by r. Then :

$$
\rho_\alpha(r) = \left(\delta_{H(u)} * {}_{\mathrm{tg}}\rho_{\alpha,u} * \Big(\operatorname*{\text{\Large$*$}}_{m=2}^{n} \delta_{\mathrm{D}_{\alpha,\lambda}^m H(u)} \Big) \right)(r) \Big|_{u=0} \ , \tag{5.1.27a}
$$

where $\delta_{H(u)}(r) = \delta\big(r - H(u)\big)$. Note that H can always be considered such that $H(0) = 0$, hence :

$$\rho_\alpha(r) = {}_{\mathrm{tg}}\rho_{\alpha,u} * \Big(\mathop{\LARGE *}_{m=2}^{n} \delta_{\mathrm{D}^m_{\alpha,\lambda} H(u)} \Big)(r) \Big|_{u=0} . \tag{5.1.27b}$$

The calculation of the Fourier transform of ρ_α is therefore simply equal to the product of the Fourier transforms of each term of the convolution product :

$$(\mathcal{F}\rho_\alpha)(k) =$$

$$= (\mathcal{F}\delta_{H(u)})(k) \, (\mathcal{F}_{\mathrm{tg}}\rho_{\alpha,u})(k) \prod_{m=2}^{n} (\mathcal{F}\delta_{\mathrm{D}^m_{\alpha,\lambda} H})(k) \Big|_{u=0} =$$

$$= \exp\big(\mathrm{i}\,k \cdot H(u)\big) \int_{\mathbb{R}^n} {}_{\mathrm{tg}}\rho_{\alpha,u}(r) \exp(\mathrm{i}\,k \cdot r)\, \mathrm{d}^n r \,\cdot$$

$$\cdot \prod_{m=2}^{n} \exp\Big(\mathrm{i}\,k \cdot \frac{1}{m!} \sum_{j_1,\ldots,j_m=1}^{n} (u_\alpha + B\,\lambda)^{j_1} \ldots (u_\alpha + B\,\lambda)^{j_m} \frac{\partial^m H(u)}{\partial u^{j_1} \ldots \partial u^{j_m}} \Big)\Big|_{u=0} .$$

This expression almost contains the exponential of the scalar product of $\mathrm{i}\,k$ and the Taylor series of H. To complete it, we multiply $(\mathcal{F}\rho_\alpha)(k)$ by

$$1 = \exp\Big(\mathrm{i}\,k \cdot \sum_{j=1}^{n} (u_\alpha + B\,\lambda)^j \frac{\partial H(u)}{\partial u^j} \Big) \exp\Big(-\mathrm{i}\,k \cdot \sum_{j=1}^{n} (u_\alpha + B\,\lambda)^j \frac{\partial H(u)}{\partial u^j} \Big)\Big|_{u=0} .$$

After simplification, we find :

$$(\mathcal{F}\rho_\alpha)(k) = \int_{\mathbb{R}^n} {}_{\mathrm{tg}}\rho_{\alpha,u}(r)\big|_{u=0} \exp(\mathrm{i}\,k{\cdot}r)\, \mathrm{d}^n r \, \exp\big(-\mathrm{i}\,k{\cdot}\Omega(0)\,(u_\alpha{+}B\,\lambda)\big) \exp\big(\mathrm{i}\,k{\cdot}H(u_\alpha{+}B\,\lambda)\big) .$$

Carrying out the change of variable $\tilde{r} - u_\alpha = r - \Omega(0)\,(u_\alpha + B\,\lambda)$, we obtain :

$${}_{\mathrm{tg}}\rho_{\alpha,u}(\tilde{r})\big|_{u=0} = \rho_\alpha(r - u_\alpha) ,$$

and :

$$(\mathcal{F}\rho_\alpha)(k) = \int_{\mathbb{R}^n} \rho_\alpha(\tilde{r} - u_\alpha) \exp(\mathrm{i}\,k \cdot \tilde{r})\, \mathrm{d}^n \tilde{r} \, \exp(-\mathrm{i}\,k \cdot u_\alpha) \exp\big(\mathrm{i}\,k \cdot H(u_\alpha + B\,\lambda)\big) =$$

$$= \exp\big(\mathrm{i}k \cdot (B\,\lambda)\big) \exp\big(\mathrm{i}\,k \cdot \tilde{H}(u_\alpha + B\,\lambda)\big) \int_{\mathbb{R}^n} \rho_\alpha(\tilde{r} - u_\alpha) \exp(\mathrm{i}\,k \cdot \tilde{r})\, \mathrm{d}^n \tilde{r} ,$$

$$\tag{5.1.28}$$

where $H = \mathrm{id} + \tilde{H}$. Summations over α and λ yield the same relation as expression 5.1.6. All these derivations can be summarised as follows.

5.1.9 Proposition : *Let $\tilde{\mathcal{S}}$ be a modulated structure (in the manifold M parameterised by H) and*

$$r \longmapsto \rho(r) = \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{n} \rho_\alpha\big(r - H(u_\alpha + B\,\lambda)\big) \ .$$

Then :

$$\rho(r) = \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{n} \left(\delta_{H(u)} *_{\mathrm{tg}}\rho_{\alpha,u} * \Big(\underset{m=2}{\overset{n}{\ast}}\ \delta_{\mathrm{D}^m_{\alpha,\lambda}H(u)} \Big) \right)(r)\bigg|_{u=0}$$

and

$$(\mathcal{F}\rho)(k) = \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{n} (\mathcal{F}\delta_{H(u)})(k)\,(\mathcal{F}_{\mathrm{tg}}\rho_{\alpha,u})(k) \prod_{m=2}^{n} (\mathcal{F}\delta_{\mathrm{D}^m_{\alpha,\lambda}H(u)})(k)\bigg|_{u=0} \ ,$$

where $_{\mathrm{tg}}\rho_{\alpha,u}$ $(_{\mathrm{tg}}\rho_{\alpha,u}|_{u=0}$ being the electron density of the atom α in the tangent space at the origin) and $\delta_{\mathrm{D}^m_{\alpha,\lambda}H(u)}$ are, respectively, given by expressions 5.1.25 and 5.1.26.

This proposition shows the connection between the electron densities on the manifold and in the tangent space at the origin, and that between the Fourier transforms of the electron densities on the manifold and in the cotangent space at the origin. This result becomes more explicit, if we write the expression of the Fourier transform of the electron density in the tangent space at the origin

$$(\mathcal{F}_{\mathrm{tg}}\rho)(k) = \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \int_{\mathbb{R}^n} \rho_\alpha\big(r - \Omega(0)\,u_\alpha\big)\exp(\mathrm{i}\,k \cdot r)\,\mathrm{d}^n r \exp\big(\mathrm{i}\,k \cdot (\Omega(0)\,B\,\lambda)\big) \ ,$$

and consider the change of variable $\tilde{r} - u_\alpha = r - \Omega(0)\,u_\alpha$. Indeed, we obtain :

$$(\mathcal{F}_{\mathrm{tg}}\rho)(k) = \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \int_{\mathbb{R}^n} \rho_\alpha\big(r - u_\alpha\big)\exp(\mathrm{i}\,k \cdot r)\,\mathrm{d}^n r \exp(-\mathrm{i}\,k \cdot u_\alpha)\exp\big(\mathrm{i}\,k \cdot (\Omega(0)\,(u_\alpha + B\,\lambda))\big) \ .$$

The substitution of $\Omega(0)\,(u_\alpha + B\,\lambda)$ by $H(u_\alpha + B\,\lambda)$ yields the Fourier transform of the electron density of the structure in the manifold. Note that the connection between $\Omega(0)\,(u_\alpha + B\,\lambda)$ and $H(u_\alpha + B\,\lambda)$ is just the Taylor series of H about 0. The summation over the terms of this series appears as a convolution product in the expression for ρ and as a product in the expression for $\mathcal{F}\rho$, as it must be, since the exponential of a sum is equal to a product of exponentials.

5.1.4 Fourier Transform and Symmetry

Let $\mathcal{S} = \{u_\alpha + B\,\lambda \mid 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n\}$ be a crystal structure in the n-dimensional Euclidean manifold endowed with the natural coordinate system, and ϕ one of its symmetry operations, the matrix and translation parts of which are, respectively, $F \in \mathrm{O}_n(\mathbb{R})$ and $s \in \mathbb{R}^n$. Since $\phi(\mathcal{S}) = \mathcal{S}$, there exists, for each α and λ, an α', $1 \leqslant \alpha' \leqslant \mu$, and a $\lambda' \in \mathbb{Z}^n$

such that $u_{\alpha'} + B\,\lambda' = F\,(u_\alpha + B\,\lambda) + s$; the atom α at $u_\alpha + B\,\lambda$ and that at $u_{\alpha'} + B\,\lambda'$ are the same. In terms of electron density, this relation between the two atoms is expressed as :

$$\rho_\alpha\big(F^{-1}\,(r - u_{\alpha'} - B\,\lambda')\big) = \rho_\alpha(r - u_\alpha - B\,\lambda)\ , \tag{5.1.30}$$

as both atoms α and α' are the same, they have the same electron density ρ_α. The role of the matrix F^{-1} is to provide the same orientation of the electron densities, in order to compare them. Taking into account the relation between u_α, $u_{\alpha'}$, λ and λ', expression 5.1.30 becomes :

$$\rho_\alpha(F^{-1}r - F^{-1}s - u_\alpha - B\,\lambda) = \rho_\alpha(r - u_\alpha - B\,\lambda)\ . \tag{5.1.31}$$

F^{-1} and $F^{-1}s$ are the matrix and translation parts of the inverse symmetry operation ϕ^{-1} of ϕ. As the derivation above holds for all symmetry operations of $\mathcal{S}$, we can conclude that

$$\rho_\alpha(F\,r + s - u_\alpha - B\,\lambda) = \rho_\alpha(r - u_\alpha - B\,\lambda)\ , \tag{5.1.32}$$

where F and s are the matrix and translation part of any symmetry operation ϕ. The summation of this expression over α and λ yields the general condition :

$$\rho(F\,r + s) = \rho(r)\ , \tag{5.1.33}$$

which figures in the International Tables for Crystallography [Shm01].

In the case of modulated structures, the symmetry of their electron density appears in a more complicated way. Compared to the average structure $\mathcal{S}$, the electron density of an atom is not only displaced, but also turned or even distorted. If

$$u \longmapsto \rho_\alpha(u - u_\alpha - B\,\lambda)$$

is the electron density of the atom α the centre of which is at the point with coordinates $u_\alpha + B\,\lambda$ in the average structure, the corresponding electron density in the modulated structure logically is :

$$r \longmapsto \rho_\alpha\big(r - H(u_\alpha + B\,\lambda)\big)\ , \quad \text{with } r = H(u)\ . \tag{5.1.34}$$

As $H(u)$ is supposed to be in a small neighbourhood of $H(u_\alpha + B\,\lambda)$, we can write :

$$H(u) = H(u_\alpha + B\,\lambda) + \Omega(u_\alpha + B\,\lambda)(u - u_\alpha - B\,\lambda) \quad \Leftrightarrow$$

$$\Leftrightarrow \quad H(u) - H(u_\alpha + B\,\lambda) = \Omega(u_\alpha + B\,\lambda)(u - u_\alpha - B\,\lambda)\ ,$$

where $\Omega = \big(\frac{\partial h^i}{\partial u^j}\big)_{i,j=1}^n$, hence :

$$\rho_\alpha\big(H(u) - H(u_\alpha + B\,\lambda)\big) = \rho_\alpha\big(\Omega(u_\alpha + B\,\lambda)(u - u_\alpha - B\,\lambda)\big) =$$

$$= \rho_\alpha\big(\Omega(u_\alpha + B\,\lambda)(H^{-1}(r) - u_\alpha - B\,\lambda)\big)\ .$$

This expression shows that ρ_α, seen as a function of the variable r, varies, for the same atom α, from one unit cell to another; the matrix field Ω gives a different orientation

according to the value of λ. The symmetry of the electron density of a whole modulated structure then appears in a more complicated way and cannot be written in a simple form, as it is the case for a structure in the Euclidean manifold (average structure).

The observed diffraction patterns of modulated structures show an invariance under the matrix part F of any symmetry operation ϕ of their corresponding average structure. A direct consequence is that main spots are transformed into main spots and satellites of order m are transformed into satellites of order $\pm m$. This implies that the modulation function H must satisfy $H(F\,u) = F\,H(u+v)$, where $v \in \mathbb{R}^n$ assures an eventual change of the phase of H. Then, we have the following result.

5.1.10 Proposition : *Let ρ be the electron density of a modulated structure $\tilde{\mathcal{S}}$ and ϕ a Euclidean symmetry operation of the corresponding average structure $\mathcal{S}$, the matrix and translation parts of which being respectively F and s. If :*

$$\left|(\mathcal{F}\rho)(F\,k)\right|^2 = \left|(\mathcal{F}\rho)(k)\right|^2 \ ,$$

then :

$$\rho(F\,r + s) = \rho(r) \ .$$

This proposition is a consequence of the properties C.3.6 of the Fourier transform (in particular the fifth and sixth). Indeed, let $T_s(\rho \circ F)(r) = \rho(F\,r + s)$; then :

$$|(\mathcal{F}\rho)(k)|^2 = |(\mathcal{F}\rho)(F\,k)|^2 \ =$$

$$= \left|\,\exp(-\mathrm{i}\,k \cdot s)\,|\det F^{-1}|(\mathcal{F}\rho)\left({}^{\mathrm{t}}(F^{-1})\,k\right)\right|^2 \ =$$

$$= \left|\left(\mathcal{F}\big(T_s(\rho \circ F)\big)\right)(k)\right|^2 \ ,$$

hence the result.   ∎

Thus, for any atom α, we have :

$$\rho_\alpha\big(F\,r + s - H(u_\alpha + B\,\lambda)\big) = \rho_\alpha\big(r - H(u_\alpha + B\,\lambda)\big) \ .$$

The left part of this relation can be written as :

$$\rho_\alpha\big(F\,r + s - H(u_\alpha + B\,\lambda)\big) = \rho_\alpha\big(F\,(r - F^{-1}H(u_\alpha + B\,\lambda) + F^{-1}s)\big) \ =$$

$$= \rho_\alpha\big(F\,(r - H(F^{-1}(u_\alpha + B\,\lambda) + F^{-1}s)\big) =$$

$$= \rho_\alpha\big(F\,(r - H(u_{\alpha'} + B\,\lambda' + v))\big) \ ,$$

where $F^{-1}(u_\alpha + B\,\lambda) = u'_\alpha + B\,\lambda' + s'$, for some α', $1 \leqslant \alpha' \leqslant \mu$, $\lambda' \in \mathbb{Z}^n$ and $s \in \mathbb{R}^n$, and $v \in \mathbb{R}^n$ is an element (phase) gathering the terms $F^{-1}s$ and s'. We then obtain :

$$\rho_\alpha\big(F\,(r - H(u_{\alpha'} + B\,\lambda' + v))\big) = \rho_\alpha\big(r - H(u_\alpha + B\,\lambda)\big) \ , \qquad (5.1.35)$$

which is an expression very similar to relation 5.1.30. It shows, in particular, that only the matrix part F of a symmetry operation of the average structure appears, and not the matrix Ω corresponding to a specific orientation of ρ_α in each unit cell. The assumption, which consists in taking the electron density of an atom α of the average structure and displacing it in the corresponding modulated structure without turning or distorting it, is therefore correct or, at least, a good approximation. In the physical reality, the electron densities in modulated structures have probably a shape adapted to the modulation, they are turned and distorted, but not so much, in such a way that the diffraction pattern presents an invariance under the matrix part of a symmetry operation of the average structure. Note that the rotation or deformation of electron densities are rather weak, because otherwise, it would mean that the modulation would have a large amplitude, and that an average structure would not correspond to the modulated structure any more.

Notice that the diffraction pattern of any non-modulated structure, that is a structure in the Euclidean manifold, is evidently also left invariant under the matrix part of any symmetry operation of the structure; this fact is a direct consequence of the properties of the Fourier transform.

The symmetry of the electron density of any modulated structure represented in a tangent space cannot be expressed through simple relations, as the electron density of each atom is not oriented according to the shape of the structure in the considered tangent space. No interesting result can be extracted, except in the Euclidean case, where the representation of a structure in any tangent space is very close to the real structure. This situation will be properly treated in the next subsection.

5.1.5 Electron Density on the Tangent Bundle

In chapter 3, a formalism extending structures and symmetry operations to the tangent bundle has been developed. The question is to know if and how this formalism can intervene in the electron density of a structure and its Fourier transform. We shall mainly discuss the Euclidean case, since the expression of symmetry operations appearing in the electron density of modulated structures cannot be simplified.

Let $\mathcal{S} = \{u_\alpha + B\,\lambda \mid 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n\}$ be a structure in the n-dimensional Euclidean manifold $\mathbb{R}^n$; the extension of $\mathcal{S}$ to $\mathrm{T}\mathbb{R}^n$ is :

$$\Xi = \{(u_\alpha + B\,\lambda - w\,;\, w) \mid 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n,\ w \in \mathbb{R}^n\}$$

or equivalently :

$$\Xi = \{(w\,;\, u_\alpha + B\,\lambda - w) \mid 1 \leqslant \alpha \leqslant \mu,\ \lambda \in \mathbb{Z}^n,\ w \in \mathbb{R}^n\}\ .$$

Let us formally write :

$$P(r;\,v) = \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} P_\alpha\big(r - w\,;\, v - (u_\alpha + B\,\lambda - w)\big)\ , \qquad (5.1.36)$$

with :

$$P_\alpha\big(r - w\,;\, v - (u_\alpha + B\,\lambda - w)\big) = \delta(r - w)\,\rho_\alpha\big(v - (u_\alpha + B\,\lambda - w)\big)\ , \qquad (5.1.37)$$

where δ is the generalised Dirac function in n dimensions. The function P can be seen as the electron density of the structure Ξ on the tangent bundle $\mathrm{T}\mathbb{R}^n$. For each $w \in \mathbb{R}^n$, it corresponds to the electron density of the structure $\mathcal{S}$ seen in the tangent space $\mathrm{T}_p\mathbb{R}^n$, where p is the point with coordinates $u_p = w$. If $w = 0$, P is the electron density of the structure in the tangent space at the origin, which is equal to that in the manifold.

The tangent bundle $\mathrm{T}\mathbb{R}^n$ corresponds to the cartesian product $\mathbb{R}^n \times \mathbb{R}^n = \mathbb{R}^{2n}$, that is $2n$ copies of $\mathbb{R}^n$ mutually orthogonal, and P is a function of the $2n$ variables $r^1, \ldots, r^n, v^1, \ldots, v^n$. Let us formally calculate its Fourier transform :

$$
\begin{aligned}
(\mathcal{F}P)(k;\,\kappa) &= \int_{\mathbb{R}^{2n}} P(r;\,v) \exp\left(\mathrm{i} \sum_{j=1}^{n} (k_j\, r^j + \kappa_j\, v^j) \right) \mathrm{d}^n r\, \mathrm{d}^n v \;= \\[2mm]
&= \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \int_{\mathbb{R}^n} \delta(r - w) \exp(\mathrm{i}\, k \cdot r)\, \mathrm{d}^n r \cdot \\[2mm]
&\qquad\qquad\qquad \cdot \int_{\mathbb{R}^n} \rho_\alpha\big(v - (u_\alpha + B\,\lambda - w)\big) \exp(\mathrm{i}\, \kappa \cdot v)\, \mathrm{d}^n v \;= \\[2mm]
&= \exp(\mathrm{i}\, k \cdot w) \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \cdot \int_{\mathbb{R}^n} \rho_\alpha(v - u_\alpha) \exp(\mathrm{i}\, \kappa \cdot v)\, \mathrm{d}^n v \cdot \\[2mm]
&\qquad\qquad\qquad\qquad\qquad \cdot \exp\big(\mathrm{i}\, \kappa \cdot (B\,\lambda)\big) \exp(-\mathrm{i}\, \kappa \cdot w) \;.
\end{aligned}
$$

Restricting this expression to the subspace $\{(k;\,\kappa) \mid k = \kappa\} \subset \mathbb{R}^{2n}$, we obtain the usual expression of the Fourier transform of the electron density ρ of a structure in $\mathbb{R}^n$. Note that :

$$
\int_{\mathbb{R}^n} P(r;\,v) \exp(\mathrm{i}\, \kappa \cdot v)\, \mathrm{d}^n r = \delta(r - w) \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \int_{\mathbb{R}^n} \rho_\alpha\big(v - (u_\alpha + B\,\lambda - w)\big) \exp(\mathrm{i}\, \kappa \cdot v)\, \mathrm{d}^n v
$$

corresponds to the Fourier transform of the electron density ρ of the structure in the tangent space at the point p with coordinates $u_p = w$. Compared to the Fourier transform of the electron density of the structure in the tangent space at the origin, it differs only by a factor $\exp(-\mathrm{i}\, k \cdot w)$. The square of the modulus of both Fourier transforms is therefore the same, implying that the diffraction pattern is exactly the same in any tangent space. This does no longer hold for modulated structures, as their shape in the tangent spaces is strongly correlated to the matrix $\Omega = \big(\frac{\partial h^i}{\partial u^j} \big)_{i,j=1}^{n}$ which depends on the considered tangent point. Notwithstanding this, the derivation above can also be carried out in the case of modulated structures, showing that defining the Fourier transform as operator from the tangent space at one point to the cotangent space at the same point is the truly natural way to proceed.

As seen previously, if $F \in \mathrm{O}_n(\mathbb{R})$ and $s \in \mathbb{R}^n$ are the matrix and translation parts of a symmetry operation ϕ of the structure $\mathcal{S}$, then $\rho(F\, r + s) = \rho(r)$. Note that this also holds in the expression of the electron density of the structure in the tangent space at the origin; F sends any vector v of the tangent space at the origin to the vector $F\, v$ in

the tangent space at the point of coordinates s, $F\,v$ corresponding to the vector $F\,v + s$ in the tangent space at the origin (see chapter 3, section 2.2). We then have :

$$\delta(r - w)\,\rho_\alpha\big(F\,v + s - (u_\alpha + B\,\lambda - w)\big) = \delta(F\,r - w)\,\rho_\alpha\big(F\,v - (u_\alpha + B\,\lambda - w - s)\big) \sim$$

$$\sim \delta(F\,r + s - w)\,\rho_\alpha\big(F\,v - (u_\alpha + B\,\lambda - w)\big)\ .$$

Thus, for the electron density in the tangent bundle, the condition $\rho(F\,r + s) = \rho(r)$ becomes :

$$P(F\,r + s\,;\,F\,v) = P(r\,;\,v)\ ; \tag{5.1.38}$$

the space group operation ϕ, represented by the matrix part F and translation part s, acts on the variables $r = (r^1;\,\ldots;\,r^n)$, while the corresponding point group operation $\mathrm{d}\phi$, represented by F, acts on the variables $v = (v^1;\,\ldots;\,v^n)$. In the Fourier transform of P, the translation part appears only in the Fourier transform of the Dirac function, which is the exponential of an imaginary number. Then, restricting $\mathcal{F}P$ to the subspace $\{(k;\,\kappa)\mid k = \kappa\}$ and taking the square of its modulus, this exponential vanishes; hence the matrix part F only, that is the point group operation only, appears in the diffraction pattern.

In conclusion, the formalism of the tangent bundle shows that the Fourier transform is naturally defined as the map $\mathcal{F} : \mathrm{T}_p\mathbb{R}^n \to \mathrm{T}_p^*\mathbb{R}^n$, and a symmetry operation ϕ carries an electron density on the tangent space $\mathrm{T}_p\mathbb{R}^n$ to an electron density on the tangent space $\mathrm{T}_{\phi(p)}\mathbb{R}^n$, where $p \in \mathbb{R}^n$. Finally, the diffraction pattern (of a non-modulated structure) is the same in any cotangent space.

5.2   Complex Electron Density on a Cylinder

The viewpoint presented in this section is more suggestive than an affirmation of reality. Its goal is to arouse a discussion about the definition of the dimension of a lattice.

5.2.1   Electron Density and Fourier Transform

If we have a look at formula 5.1.7, we notice that the integration is carried out over one unit cell only; moreover, in any function ρ_α the position of the atom α in the average structure appears. Let us introduce a new degree of freedom r^{n+1} and formally write :

$$Q(r;\,r^{n+1}) = \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha)\exp\big(\mathrm{i}\,k \cdot \tilde{H}(r^{n+1} + \xi \cdot u_\alpha)\big)\ , \tag{5.2.1a}$$

$$\delta_{\Lambda^{n+1}}(r) = \sum_{\lambda \in \mathbb{Z}^n} \delta\big(r - B\,\lambda\big)\,\delta\big(r^{n+1} + \xi \cdot (B\,\lambda)\big)\ . \tag{5.2.1b}$$

The convolution product of Q and $\delta_{\Lambda^{n+1}}$ is :

$$(Q * \delta_{\Lambda^{n+1}})(r;\, r^{n+1}) \;=\; \int_{\mathbb{R}^{n+1}} \sum_{\alpha=1}^{\mu} \rho_\alpha(r - r' - u_\alpha) \exp\big(\mathrm{i}\, k \cdot \tilde{H}(r^{n+1} - r'^{n+1} + \xi \cdot u_\alpha)\big) \cdot$$

$$\cdot \sum_{\lambda \in \mathbb{Z}^n} \delta(r' - B\,\lambda)\, \delta\big(r'^{n+1} + \xi \cdot (B\,\lambda)\big)\, \mathrm{d}^n r'\, \mathrm{d} r'^{n+1} =$$

$$= \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha - B\,\lambda)\, \exp\big(\mathrm{i}\, k \cdot \tilde{H}(r^{n+1} + \xi \cdot (u_\alpha + B\,\lambda))\big) \; ; \tag{5.2.2}$$

restricting this expression to the subspace $\{r = (r^1;\, \ldots;\, r^n;\, r^{n+1}\} \in \mathbb{R}^{n+1} \mid r^{n+1} = 0\}$, we obtain :

$$(Q * \delta_{\Lambda^{n+1}})(r;\, 0) = \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha - B\,\lambda)\, \exp\big(\mathrm{i}\, k \cdot \tilde{H}(\xi \cdot (u_\alpha + B\,\lambda))\big) \;, \tag{5.2.3}$$

the Fourier transform of which is, with respect to the usual variables $r = (r^1;\, \ldots;\, r^n)$:

$$\big(\mathcal{F}(Q * \delta_{\Lambda^{n+1}})|_{\mathbb{R}^n \times \{0\}}\big)(k) =$$

$$= \int_{\mathbb{R}^n} \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha - B\,\lambda)\, \exp\big(\mathrm{i}\, k \cdot \tilde{H}(\xi \cdot (u_\alpha + B\,\lambda))\big) \exp(\mathrm{i}\, k \cdot r)\, \mathrm{d}^n r \;=$$

$$= \int_{\mathbb{R}^n} \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha - B\,\lambda)\, \exp(\mathrm{i}\, k \cdot r)\, \mathrm{d}^n r\, \exp\big(\mathrm{i}\, k \cdot \tilde{H}(\xi \cdot (u_\alpha + B\,\lambda))\big) \;=$$

$$= \int_{\mathbb{R}^n} \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(\tilde{r} - u_\alpha)\, \exp(\mathrm{i}\, k \cdot \tilde{r})\, \mathrm{d}^n \tilde{r}\, \exp\big(\mathrm{i}\, k \cdot (B\,\lambda)\big) \exp\big(\mathrm{i}\, k \cdot \tilde{H}(\xi \cdot (u_\alpha + B\,\lambda))\big) \;. \tag{5.2.4}$$

It corresponds to the Fourier transform of the electron density of a modulated structure $\tilde{\mathcal{S}}$ (see expression 5.1.6). Note that the parameter $k \in \mathbb{R}^n$ appearing in $\exp(\mathrm{i}\, k \cdot r)$ of the Fourier transform is the same as that of Q; two different characters k and $\tilde{k}$ could also be used and the condition $k = \tilde{k}$ on the final expression could then be applied.

Let us focus on the function $\tilde{H}$. According to a previous hypothesis, it is a periodic wave function of the position, that is $\tilde{H}(\xi \cdot r + \bar{T}) = \tilde{H}(\xi \cdot r)$, where $\bar{T} = T\,\|\xi\|$, $T \in \mathbb{R}_+^*$. Thus, $\tilde{H}$ and therefore $\exp(\mathrm{i}\, k \cdot \tilde{H})$, seen as a function of the variable r^{n+1}, can be restricted to the interval $[0\,;\, \bar{T}[$. Let $[\xi \cdot (B\,\lambda)] \in [0\,;\, \bar{T}[$ such that $[\xi \cdot (B\,\lambda)] = \xi \cdot (B\,\lambda) + m\,\bar{T}$, for an $m \in \mathbb{Z}$, $\bar{Q}$ and $\bar{\delta}_{\Lambda^{n+1}}$ the functions given, respectively, by :

$$\bar{Q}(r;\, r^{n+1}) = \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha)\, \exp\big(\mathrm{i}\, k \cdot \tilde{H}(r^{n+1} + \xi \cdot u_\alpha)\big) \;, \tag{5.2.5a}$$

$$\bar{\delta}_{[\Lambda^{n+1}]} = \sum_{\lambda \in \mathbb{Z}^n} \delta(r - B\,\lambda)\, \delta\big(r^{n+1} + [\xi \cdot (B\,\lambda)]\big) \;, \tag{5.2.5b}$$

corresponding to the functions Q and $\delta_{\Lambda^{n+1}}$ restricted to the domain $\mathbb{R}^n \times [0\,;\bar{T}[$. Their convolution product is :

$$
(\bar{Q} * \bar{\delta}_{[\Lambda^{n+1}]})(r;\,r^{n+1}) \;\;=\;\; \int\limits_{\mathbb{R}^n \times [0\,;T']} \sum_{\alpha=1}^{\mu} \rho_\alpha(r - r' - u_\alpha)\exp\!\big(\mathrm{i}\,k\cdot\tilde{H}(r^{n+1} - r'^{n+1} + \xi\cdot u_\alpha)\big) \cdot
$$

$$
\cdot \sum_{\lambda\in\mathbb{Z}^n}\delta(r' - B\,\lambda)\,\delta(r'^{n+1} + [\xi\cdot(B\,\lambda)])\,\mathrm{d}^n r'\,\mathrm{d}r'^{n+1} =
$$

$$
= \sum_{\lambda\in\mathbb{Z}^n}\sum_{\alpha=1}^{\mu}\rho_\alpha(r - u_\alpha - B\,\lambda)\,\exp\!\big(\mathrm{i}\,k\cdot\tilde{H}(r^{n+1} + [\xi\cdot(B\,\lambda)] + \xi\cdot u_\alpha)\big)\,,
$$

$$
(5.2.6)
$$

where the integration domain is $\mathbb{R}^n \times [0\,;\bar{T}[$. This expression is equal to formula 5.2.2. Indeed, as $\tilde{H}$ is periodic, then :

$$
\tilde{H}(r^{n+1} + [\xi\cdot(B\,\lambda)] + \xi\cdot u_\alpha) = \tilde{H}(r^{n+1} + \xi\cdot(B\,\lambda) + m\,T' + \xi\cdot u_\alpha) =
$$

$$
= \tilde{H}(r^{n+1} + \xi\cdot(B\,\lambda) + \xi\cdot u_\alpha)\,.
$$

The periodicity of $\tilde{H}$ suggests that we may think of the domain $\mathbb{R}^n \times [0\,;\bar{T}[$ as a cylinder $\mathcal{C}^{n+1}$ of dimension $n+1$ which can be embedded in the Euclidean space $\mathbb{R}^{n+2}$ and therefore parameterised by the map :

$$
\mathbb{R}^{n+1} \qquad\qquad \longrightarrow \qquad\qquad\qquad \mathbb{R}^{n+2}
$$

$$
(r^1;\,\ldots;\,r^n;\,r^{n+1}) \;\;\longmapsto\;\; \left(r^1;\,\ldots;\,r^n;\,\frac{\bar{T}}{2\,\pi}\cos\!\Big(\frac{2\,\pi\,r^{n+1}}{\bar{T}}\Big);\,\frac{\bar{T}}{2\,\pi}\sin\!\Big(\frac{2\,\pi\,r^{n+1}}{\bar{T}}\Big)\right)\;\;.
$$

Since the components of the metric tensor associated with this parameterisation are :

$$
g_{ij} = \delta_{ij}\,, \qquad\qquad\qquad\qquad\qquad\qquad 1 \leqslant i,j \leqslant n\,,
$$

$$
g_{i,n+1} = g_{n+1,i} = \frac{\partial r^i}{\partial r^{n+1}} = 0\,, \qquad\qquad\qquad 1 \leqslant i \leqslant n\,,
$$

$$
g_{n+1,n+1} = \sin^2\!\Big(\frac{2\,\pi\,r^{n+1}}{\bar{T}}\Big) + \cos^2\!\Big(\frac{2\,\pi\,r^{n+1}}{\bar{T}}\Big) = 1\,,
$$

that is :

$$
g_{ij} = \delta_{ij}\,, \qquad 1 \leqslant i,j \leqslant n+1\,,
$$

$\mathcal{C}^{n+1}$ is a smooth manifold which has the same geometrical properties as the Euclidean space. The functions $\bar{Q}$ and $\bar{\delta}_{\Lambda^{n+1}}$ are then nothing but the expression of Q and $\delta_{\Lambda^{n+1}}$ on $\mathcal{C}^{n+1}$. Indeed, as the radius of $\mathcal{C}^{n+1}$ is equal to $\frac{\bar{T}}{2\,\pi}$, the circumference of its basis is equal to $\bar{T}$, the periodicity of the function $\tilde{H}$.

5.2.1 Proposition : *The electron density of any modulated structure in a manifold of dimension n, with one modulation function (i.e. with one wave vector), can be*

interpreted as a complex electron density of a structure on a cylinder $\mathbb{C}^{n+1}$ of dimension $n+1$. Moreover, according to expressions 5.2.5a and 5.2.5b, this electron density can be written as a convolution product of the electron density $\bar{Q}$ over one unit cell and the Dirac function $\delta_{\Lambda^{n+1}}$ of a lattice on $\mathbb{C}^{n+1}$, projected on the submanifold $\{(r;\ r^{n+1}) \mid r^{n+1} = 0\}$.

5.2.2 Remark : The projection on the axis of the coordinate r^{n+1} of all points of the lattice $\Lambda^{n+1} = \left\{(B\,\lambda\,;\, \xi\cdot(B\,\lambda)) \mid \lambda \in \mathbb{Z}^n\right\} \subset \mathbb{C}^{n+1}$ constitutes a dense set in the interval $[0\,;\, \bar{T}[$ if and only if $\xi\cdot(B\,\lambda) \neq q\,\bar{T}$, where $q \in \mathbb{Q}$ is a rational number, for one $\lambda \in \mathbb{Z}^n$ at least.

5.2.2 A Question about the Dimension of a Lattice

Let us consider the example of a one-dimensional modulated structure, the electron density of which is :

$$\rho(r) = \sum_{\lambda\in\mathbb{Z}} \sum_{\alpha=1}^{\mu} \rho_\alpha\big(r - u_\alpha - b\,\lambda - \tilde{h}(u_\alpha + b\,\lambda)\big)\ ,$$

where r is a one-dimensional variable, u_α the coordinate of the atom α, $b > 0$ the cell parameter characterising the lattice $\{b\,\lambda \mid \lambda \in \mathbb{Z}\}$ and $\tilde{h}$ the one-dimensional modulation function, that is a wave function of the position, $r \mapsto \tilde{h}(\xi\,r)$, where $\xi \in \mathbb{R}$ is the wave vector. Let us write :

$$Q(r;\ \tilde{r}) = \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha)\exp\big(\mathrm{i}\,k\,\tilde{h}(\tilde{r} + \xi\,u_\alpha)\big)\ ,$$

$$\delta_{\Lambda^2}(r;\ \tilde{r}) = \sum_{\lambda\in\mathbb{Z}} \delta(r - b\,\lambda)\,\delta(\tilde{r} + \xi\,b\,\lambda)\ ,$$

According to the considerations of the previous subsection, the convolution product of Q and δ_{Λ^2} restricted to the subspace $\{(r;\ \tilde{r}) \in \mathbb{R}^2 \mid \tilde{r} = 0\}$ and ρ are equivalent in the sense that both have the same Fourier transform. The set $\Lambda^2 = \{(b\,\lambda;\ \xi\,b\,\lambda) \mid \lambda \in \mathbb{Z}\}$ associated with the Dirac function δ_{Λ^2} is a one-dimensional lattice in $\mathbb{R}^2$, which has the structure of a finite free $\mathbb{Z}$-module (see figure 5.1).

As $\tilde{h}$ is periodic, there exists a $\bar{T} \in \mathbb{R}_+^*$ such that $\tilde{h}(\tilde{r} + \xi\,u_\alpha + \bar{T}) = \tilde{h}(\tilde{r} + \xi\,u_\alpha)$. Let $m \in \mathbb{Z}$ such that $[\xi\,b\,\lambda] = \xi\,b\,\lambda + m\,\bar{T} \in [0\ \bar{T}[$. The convolution product of the two functions $\bar{Q}$ and $\bar{\delta}_{\Lambda^2}$ given by :

$$\bar{Q}(r;\ \tilde{r}) = \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha)\exp\big(\mathrm{i}\,k\,\tilde{h}(\tilde{r} + \xi\,u_\alpha)\big)\ ,$$

$$\bar{\delta}_{[\Lambda^2]}(r;\ \tilde{r}) = \sum_{\lambda\in\mathbb{Z}} \delta(r - b\,\lambda)\,\delta(\tilde{r} + [\xi\,b\,\lambda])\ ,$$
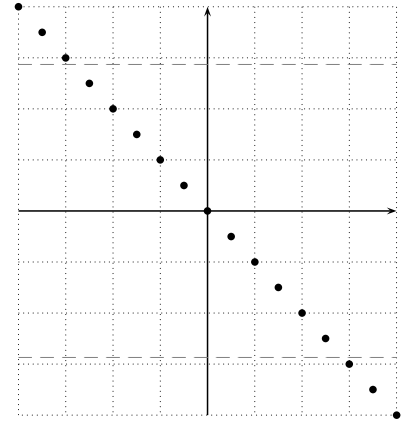

Figure 5.1: One-dimensional lattice in $\mathbb{R}^2$.

where $\tilde{r} \in [0\,;\bar{T}[$, is then equal to the convolution product of Q and δ_{Λ^2}.

Let us concentrate on the lattice

$$[\Lambda^2] = \{(b\,\lambda;\,[\xi\,b\,\lambda]) \mid \lambda \in \mathbb{Z}\}$$

associated with the Dirac function $\bar{\delta}_{[\Lambda^2]}$. On the one hand, it still looks like a one-dimensional finite free $\mathbb{Z}$-module, especially when $\mathbb{R}\times[0\,;\bar{T}[$ is seen as a cylinder. On the

Figure 5.2: A one-dimensional lattice in the domain $\mathbb{R} \times [0\,;\bar{T}[$, or equivalently on a cylinder, looks like a two-dimensional lattice.

other hand, it can also be considered as a two-dimensional lattice. Figure 5.2 illustrates the situation; we clearly see that the unit cell can be a segment as well as a two dimensional parallelogram. Note that this also holds in the case of a non-modulated structure. Indeed, in such a case, the lattice is just $\{(b\,\lambda;\,[0]) \mid \lambda \in \mathbb{Z}\}$, which can be seen as a two-dimensional lattice as well. Such a situation appears every time when one or more dimensions are compact, as it is the case on a cylinder.
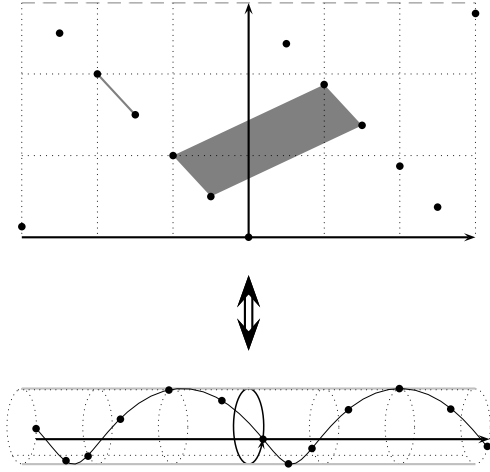
This one-dimensional example can be extended to n-dimensional modulated structures. But instead of adding only one degree of freedom, as it has been done in the previous subsection, we introduce n new variables $\tilde{r}^1,\ldots,\tilde{r}^n$. Q and $\delta_{\Lambda^{2n}}$ becomes functions of $2\,n$ variables :

$$Q(r;\,\tilde{r}) = \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha)\exp\big(\mathrm{i}\,k\cdot\tilde{H}(\xi\cdot(\tilde{r}+u_\alpha))\big)\ ,$$

$$\delta_{\Lambda^{2n}}(r;\,\tilde{r}) = \sum_{\lambda\in\mathbb{Z}^n} \delta(r - B\,\lambda)\,\delta(\tilde{r}+B\,\lambda)\ .$$

Let $m = (m^1;\,\ldots;\,m^n)$ be the element of $\mathbb{Z}^n$ such that

$$[B\,\lambda] \;=\; \big([(B\,\lambda)^1];\,\ldots;\,[(B\,\lambda)^n]\big) \;=$$

$$=\; \left((B\,\lambda)^1 + \frac{m^1\,\bar{T}}{\xi^1};\,\ldots;\,(B\,\lambda)^n + \frac{m^n\,\bar{T}}{\xi^n}\right) \;\in\; \left[0;\,\frac{\bar{T}}{\xi_1}\right[\times \ldots \times \left[0;\,\frac{\bar{T}}{\xi_n}\right[\ ,$$

where $\xi = (\xi^1;\,\ldots;\,\xi^n)$, and let

$$\bar{\bar{Q}}(r;\,\tilde{r}) = \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha)\exp\big(\mathrm{i}\,k\cdot\tilde{H}(\xi\cdot(\tilde{r}+u_\alpha))\big)\ ,$$

$$\bar{\bar{\delta}}_{[\Lambda^{2n}]}(r;\,\tilde{r}) = \sum_{\lambda\in\mathbb{Z}^n} \delta(r - B\,\lambda)\,\delta(\tilde{r}+[B\,\lambda])\ .$$

be, respectively, the two functions Q and $\delta_{\Lambda^{2n}}$ restricted to the domain

$$\mathcal{D} \doteq \mathbb{R} \times \cdots \times \mathbb{R} \times \left[0\,;\,\frac{\bar{T}}{\xi_1}\right[\times \ldots \times \left[0\,;\,\frac{\bar{T}}{\xi_n}\right[\quad .$$

Then :

$$\left(\bar{\bar{Q}} * \bar{\bar{\delta}}_{[\Lambda^{2n}]}\right)(r;\,\tilde{r}) \;=\; \int_{\mathcal{D}} \sum_{\alpha=1}^{\mu} \rho_\alpha(r - r' - u_\alpha) \exp\!\big(\mathrm{i}\,k \cdot \tilde{H}(\xi \cdot (\tilde{r} - \tilde{r}' + u_\alpha)))\big) \cdot$$

$$\cdot \sum_{\lambda \in \mathbb{Z}^n} \delta(r' - B\,\lambda)\, \delta(\tilde{r}' + [B\,\lambda])\, \mathrm{d}^n r'\, \mathrm{d}^n \tilde{r}' \;=$$

$$=\; \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha - B\,\lambda) \exp\!\big(\mathrm{i}\,k \cdot \tilde{H}(\xi \cdot (\tilde{r} + u_\alpha + [B\,\lambda])))\big) \;=$$

$$=\; \sum_{\lambda \in \mathbb{Z}^n} \sum_{\alpha=1}^{\mu} \rho_\alpha(r - u_\alpha - B\,\lambda) \exp\!\big(\mathrm{i}\,k \cdot \tilde{H}(\xi \cdot (\tilde{r} + u_\alpha + B\,\lambda)))\big) \;,$$

as :

$$\xi \cdot [B\,\lambda] = \sum_{j=1}^{n} \xi_j \,[(B\,\lambda)^j] = \sum_{j=1}^{n} \xi_j \left((B\,\lambda)^j + \frac{m^j\,\bar{T}}{\xi_j}\right) = \sum_{j=1}^{n} \xi_j\,(B\,\lambda)^j + \sum_{j=1}^{n} m^j\,\bar{T} \;.$$

We find again expression 5.2.2. In conclusion, with each variable r^i, a variable r'^i can be associated the values of which lie in the interval $\left[0\,;\,\frac{\bar{T}}{\xi^i}\right[$. Each dimension of $\mathbb{R}^n$ can then be seen as a rope resembling a thread from a distance and a two-dimensional object from near. The set $\Lambda^{2n} = \{(B\,\Lambda;\,[B\,\Lambda]) \mid \lambda \in \mathbb{Z}^n\}$, which can be seen as an n-dimensional, as well as a $2n$-dimensional lattice, looks like a normal n-dimensional lattice from a distance. Similar considerations appear in cosmology, more precisely in the braneworld formalism (see for instance articles [Lan02, DK04]).

Outlook

Differential geometry and Lie groups offer an appropriate framework for studying the geometrical and symmetrical features of crystals, whether modulated or not. Using the right tools in appropriate spaces, concepts such as *point group* and *space group* appear in a more natural way, without requiring additional dimensions in the modulated case. Thanks to the concept of tangent spaces, a symmetry operation may be represented in two different ways : as a map in a manifold or as a linear map between two tangent spaces. Combining these two viewpoints, one obtains a representation of symmetry operations which is independent of any choice of origin. Such a formulation is particularly useful if the symmetry elements associated with different operations do not all intersect in one point.

A point open to criticism is that the position of atoms in the tangent space does not necessarily correspond to their real position in a structure. However, as a one-to-one correspondance between vectors in the tangent space and points in the manifold always exists, a vector in a tangent space automatically defines a point in the manifold. Moreover, the representation of modulated structures in superspace does not correspond to physical reality either, as the positions of atoms are not points but lines, surfaces or volumes; the real three-dimensional structure is obtained by taking a section of the superspace structure.

The translation group, seen as a Lie group, is an essential tool for describing the periodicity of a crystal. Any crystal structure, whether modulated or not, is obtained by the application of a discrete subgroup of the translation group to the points of a (decorated) unit cell. The translation group is the instrument which generates the three-dimensional repetition of a brick, while taking into account the particular geometry of the space in which the cell is considered. Thus, the Fourier transform of the electron density of a modulated structure can be written as the Fourier transform of the electron density over one (modulated) unit cell on which acts a discrete subgroup of translations. The notion of *structure factor* is then recovered in modulated structures, without using additional dimensions.

In the light of the presented results, three tracks would merit further exploration. First, one should try to solve and refine a modulated structure by using the concept of action of the translation group on the electron density over a unit cell. As the structure factor can be isolated in the expression of the Fourier transform of the electron density of a modulated structure, this should be possible somehow, even if the action of the elements of the translation group on a point does not consist in a multiplication but involve the concept of derivative. Second, one should consider a modulated structure in

a real curved space and not in the Euclidean space endowed with a curved coordinate system. Then, a modulated structure and its corresponding average structure would be a unique crystal the modulated aspect of which would depend on the point of the space from which it would be observed. Finally, the model which describes a crystal in a cylinder would merit some more investigations. The only information about a crystal one has at the atomic scale is the diffraction pattern, which can be subject to different interpretations. Thus, one does not directly know the properties of a real structure, one can only make assumptions more or less compatible with the observations. One can then wonder if there are not any other phenomena which might cause the satellite spots appearing in some diffraction patterns. . .

Appendix A

Notation and Terminology

Nomenclature often used throughout this work :

M	manifold
$\mathcal{U}, \mathcal{U}'$	open sets
$(\mathcal{U}; \varphi)$	coordinate system
p, q	points
v, w	vectors
γ	curve
$\mathcal{G}$	Lie group
$\mathfrak{g}$	Lie algebra

Most frequently used matrice sets :

$\mathrm{M}_n(\mathbb{R})$	ring of real $n \times n$ matrices
$\mathrm{GL}_n(\mathbb{R})$	group of all real invertible $n \times n$ matrices, called *full linear group*
$\mathrm{O}_n(\mathbb{R})$	group of all (real) orthogonal $n \times n$ matrices, called *orthogonal group*
$\mathrm{SO}_n(\mathbb{R})$	subgroup of all (real) orthogonal $n \times n$ matrices with determinant $+1$
$\mathrm{GL}_n(\mathbb{Z})$	subset of all (real) invertible $n \times n$ matrices with integer components
$\mathrm{O}_n(\mathbb{Z})$	subgroup of all orthogonal $n \times n$ matrices with integer components
$\mathrm{SO}_n(\mathbb{Z})$	subgroup of all matrices of $\mathrm{SO}_n(\mathbb{R})$ with integer components

The sign $\doteq$ expresses a definition. For instance, $a_i \doteq \sum_{j=1}^{n} b^j{}_i \, e_j$ means that a_i is defined as $\sum_{j=1}^{n} b^j{}_i \, e_j$.

The *Kronecker symbol* is the symbol δ_{ij}, where i and j are indexes, wich takes the value 1 if $i = j$, and which is equal to 0 otherwise. Several notations are used, according to the tensor notations and conventions :

$$\delta_{ij} \ , \qquad \delta^{ij} \ , \qquad \delta^i{}_j \ .$$

In general, δ_{ij} and δ^{ij} correspond to the component $(i; j)$ of the scalar product on any tangent and cotangent spaces of the Euclidean manifold, respectively, while $\delta^i{}_j$ appears in the duality between these two spaces.

The transpose of a matrix A is noted ${}^t\!A$. Its inverse, when it exists, is A^{-1}. A matrix U is orthogonal if ${}^t\!U\,U = I_n$, where I_n is the $n \times n$ identity matrix. A matrix $\operatorname{diag}(a_1; a_2; \ldots; a_n)$ is a diagonal matrix with the values $a_1, a_2, \ldots, a_n \in \mathbb{R}$ in the diagonal. For practical and aesthetic reasons, this notation is often used inside a text.

A vector v in an n-dimensional vector space V can be written $v = \sum_{j=1}^{n} v^j\,e_j$, where $e_1, \ldots, e_n$ form a basis of V. Equivalent notations for v are :

$$
v = \begin{pmatrix} v^1 \\ \vdots \\ v^n \end{pmatrix} \qquad \text{or} \qquad v = (v^1; \ldots; v^n) \, .
$$

The first expression is a matrix notation of v; the vector is written as an $n \times 1$ matrix, called *column-vector*. The second one expresses exactly the same, it corresponds to v in the column-vector notation. It is used inside a text, for practical reasons. It is *neither* a matrix notation, *nor* an $1 \times n$ matrix, *nor* the transposed matrix of the column-vector,

$$
\begin{pmatrix} v^1 & \ldots & v^n \end{pmatrix} \neq (v^1; \ldots; v^n) \, .
$$

The norm of a vector v is noted $\|v\|$; the modulus of a complex number z is $|z|$.

A $\mathbb{Z}$-module is an abelian group $\mathcal{G}$ furnished with an external operation (multiplication) which is distributive, associative and for which a neutral element exists. A *finite free module* over the ring of integer numbers $\mathbb{Z}$ is a $\mathbb{Z}$-module which is isomorphic to $\mathbb{Z}^n$, for a certain $n \in \mathbb{N} \smallsetminus \{0\}$. The number n is called the dimension of the module; this latter is said to be of dimension n.

For a manifold of dimension n, the map φ of a coordinate system $(\mathcal{U}; \varphi)$ can be written as an n-tuple $\varphi = (x^1; \ldots; x^n)$. The alternative notation $x = (x^1; \ldots; x^n)$ is often used, too. If the neighbourhood $\mathcal{U}$ can be extended to the whole manifold, the coordinate system is noted simply φ, or x, and $\mathcal{U}$ is omitted.

$\mathbb{R}^n$ is referred to several different objects. It is first the cartesian product of n copies of the field of real numbers $\mathbb{R}$. Elements of $\mathbb{R}^n$ are then all n-tuples $a = (a^1; \ldots; a^n)$ of real numbers. Addition rule of two n-tuples, $a + b = (a^1; \ldots; a^n) + (b^1; \ldots; b^n) = (a^1 + b^1; \ldots; a^n + b^n)$, and multiplication by a real number $\mu \in \mathbb{R}$, $\mu\,a = \mu\,(a^1; \ldots; a^n) = (\mu\,a^1; \ldots; \mu\,a^n)$ make of $\mathbb{R}^n$ a vector space. The n vectors $(1; 0; \ldots; 0), (0; 1; \ldots; 0), \ldots, (0; 0; \ldots; 1)$ constitute a basis of this vector space, which is called *canonical basis* of $\mathbb{R}^n$. Endowing $\mathbb{R}^n$ with the scalar product $\cdot$, given by $a \cdot b = (a^1\,b^1; \ldots; a^n\,b^n)$ and known as *Euclidean scalar product*, notions of angle and length can be introduced. $\mathbb{R}^n$ can then be seen as a metric space, hence a topological space; the metric function is given by $\operatorname{dist}(a; b) = \sqrt{(a - b) \cdot (a - b)}$ and the topological concept of open set is based on this function. Thus, $\mathbb{R}^n$ may be referred to an n-dimensional manifold. The identity map $\operatorname{id} : \mathbb{R}^n \to \mathbb{R}^n$ constitutes a coordinate system of the whole space $\mathbb{R}^n$. For each $1 \leqslant i \leqslant n$, consider the function u^i sending any point p of $\mathbb{R}^n$, that is any n-tuple $a_p = (a_p{}^1; \ldots; a_p{}^n)$ to $a_p{}^i$; then, the n-tuple of functions $(u^1; \ldots; u^n)$ carries $a_p = (a_p{}^1; \ldots; a_p{}^n)$ into itself. $u^1, \ldots, u^n$ are called *natural coordinate functions* and $(\mathbb{R}^n; u)$, where $u = (u^1; \ldots; u^n)$, is called *natural coordinate system*. As a consequence of the definition of the *Euclidean scalar product*, the components of

the metric tensor in $(\mathbb{R}^n; u)$ are $g_{ij} = \delta_{ij}$, for all $1 \leqslant i, j \leqslant n$, where δ_{ij} is the *Kronecker symbol*. Taking this property as a definition of the natural coordinate system, one has not only one but an infinity of possible natural coordinate systems. $\mathbb{R}^n$ furnished with a natural coordinate system is called *Euclidean manifold*.

A topological space $\mathcal{T}$ is said to be Hausdorff, or separate, if for any two different points $p_1, p_2 \in \mathcal{T}$, there exists open neighbourhoods $\mathcal{U}_1 \subset \mathcal{T}$ of p_1 and $\mathcal{U}_2 \subset \mathcal{T}$ of p_2 such that $\mathcal{U}_1 \cap \mathcal{U}_2 = \varnothing$.

A map $f : M_1 \to M_2$ is *injective* if $p \neq q$, $p, q \in M_1$, implies $f(p) \neq f(q)$. It is *surjective* if its image $\{f(p) \mid p \in M_1\}$ is equal to M_2. A map f which is injective and surjective is said to be *one-to-one*. Its inverse map exists and is noted f^{-1}. The map f is called a *homeomorphism* if it is one-to-one, continuous, and if its inverse is also continuous. Moreover, if f is a *smooth* homeomorphism, the inverse of which is also *smooth*, it is called a *diffeomorphism*.

A real-valued function f defined on an open set $\mathcal{U} \in \mathbb{R}^n$ is said to be *smooth*, or equivalently $C^\infty(\mathcal{U})$, provided that all its derivatives of all orders exist and are continuous in $\mathcal{U}$.

In this work, the considered manifolds are always embedded in $\mathbb{R}^n$, where $n \in \mathbb{N}$. Their dimension is then $m \in \mathbb{N}$, with $m \leqslant n$; their topology and metric are induced by those of $\mathbb{R}^n$. Moreover, any point p of M, the coordinates of which are $\varphi(p) = (x_p{}^1; \ldots; x_p{}^m)$ in a coordinate system $(\mathcal{U}; \varphi)$, $p \in \mathcal{U} \subset M$, can also be seen as a point of $\mathbb{R}^n$ with coordinates $u_p = (u_p{}^1; \ldots; u_p{}^n)$, where $(\mathbb{R}^n; u)$ is the natural coordinate system.

The term *representation* is used in different meanings. In many cases, it does not have a particular mathematical meaning, except in the context of algebraic groups, where it corresponds to the group homomorphism between the considered group and the group of invertible matrices R or elements $(R; s)$, where $s \in \mathbb{R}^n$.

More information, as well as useful formulae, may be found in the *Oxford User's Guide to Mathematics* [gm04].

Appendix B

Lie Groups

An overview of this mathematical topic is presented; main definitions and results are mentioned without proofs. More information can be obtained in the textbooks of B. O'Neill [O'N83], D. H. Sattinger and O. L. Weaver [DHS86], and V. S. Varadarajan [Var84], for instance.

B.1 Generalities

B.1.1 Definition : Let $(\mathcal{G}; \diamond)$ be a group with internal composition operation $\diamond$ and neutral element e. $\mathcal{G}$ is a *Lie group* if it is also a smooth manifold and if the operations

$$\diamond : \begin{aligned} \mathcal{G} \times \mathcal{G} &\longrightarrow \mathcal{G} \\ (g_1; g_2) &\longmapsto g_1 \diamond g_2 , \end{aligned}$$

and

$$\begin{aligned} \mathcal{G} &\longrightarrow \mathcal{G} \\ g &\longmapsto g^{-1} , \end{aligned}$$

where $g^{-1} \diamond g = g \diamond g^{-1} = e$ are both smooth.

A Lie group can then be parameterised by some real independent parameters. Their number gives the dimension of the manifold.

B.1.2 Example : The set of real $n \times n$ matrices $\mathrm{M}_n(\mathbb{R})$ is a group with respect to addition but not multiplication. It can be seen, in a natural way, as the space $\mathbb{R}^{n^2}$, which is a manifold. Since the determinant is a smooth function, the subset $\mathrm{GL}_n(\mathbb{R})$ of all $n \times n$ invertible matrices is a submanifold of $\mathrm{M}_n(\mathbb{R})$. It is also a group with respect to matrix multiplication. As the multiplication and inverse operations are smooth functions, then $\mathrm{GL}_n(\mathbb{R})$ is a Lie group.

B.1.3 Proposition : *Let $\mathcal{H}$ be a closed subgroup of a Lie group $\mathcal{G}$, that is a subgroup which is a closed set of $\mathcal{G}$. Then $\mathcal{H}$ is a submanifold of $\mathcal{G}$. This implies that $\mathcal{H}$ has the structure of a Lie group, it is a Lie subgroup of $\mathcal{G}$.*

B.2 Lie Algebras

B.2.1 Definition : A *Lie algebra* over the field $\mathbb{R}$ is a real vector space $\mathfrak{g}$ furnished with a bilinear function $[\ \ ;\ \ ] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$, called *Lie bracket operation*, satisfying the two requirements :

- skew-symmetry :
$$[X; Y] = -[Y; X] \ , \quad \forall\, X, Y \in \mathfrak{g} \ ,$$

- Jacobi identity :
$$\big[[X; Y]; Z\big] + \big[[Y; Z]; X\big] + \big[[Z; X]; Y\big] = 0 \ , \quad \forall\, X, Y, Z \in \mathfrak{g} \ .$$

B.2.2 Example : The set of all real $n \times n$ matrices $\mathrm{M}_n(\mathbb{R})$ is a vector space. The commutator $[A; B] = A\,B - B\,A$ of two matrices is an operation which satisfies the skew-symmetry property and Jacobi identity. Thus, $\mathrm{M}_n(\mathbb{R})$ is a Lie algebra.

B.2.3 Definition : Let $\mathcal{G}$ be a Lie group (with internal composition operation $\diamond$) . For $a \in \mathcal{G}$, let us consider the maps $\mathcal{L}_a$ and $\mathcal{R}_a$ given respectively by $\mathcal{L}_a(g) = a \diamond g$ and $\mathcal{R}_a = g \diamond a$, for all $g \in \mathcal{G}$. Let $\mathrm{d}\mathcal{L}_a$ and $\mathrm{d}\mathcal{L}_a$ be their respective differential map at a. A vector field Y on $\mathcal{G}$ is said to be *left-invariant*, respectively *right-invariant*, provided $\mathrm{d}\mathcal{L}_a(Y) = Y$, respectively $\mathrm{d}\mathcal{R}_a(Y) = Y$, for all $a \in \mathcal{G}$. Explicitly, $\mathrm{d}\mathcal{L}_a(Y_g) = Y_{a \diamond g}$ and $\mathrm{d}\mathcal{R}_a(Y_g) = Y_{g \diamond a}$, for all $a, g \in \mathcal{G}$.

B.2.4 Remark : $\mathcal{L}_a$ and $\mathcal{R}_a$ are diffeomorphisms. Indeed, they are smooth and they possess the inverses $\mathcal{L}_{a^{-1}}$ and $\mathcal{R}_{a^{-1}}$, respectively.

B.2.5 Proposition : *Let $\mathfrak{l}$ be the set of all left-invariant vector fields on a Lie group $\mathcal{G}$. Then $\mathfrak{l}$ is a Lie algebra, called* Lie algebra of $\mathcal{G}$. *Henceforth, it will be written $\mathfrak{g}$.*

Indeed, the usual addition of vector fields and multiplication by a real number make $\mathfrak{l}$ a vector space. Moreover, $\mathfrak{l}$ is closed under the $[\ \ ;\ \ ]$ operation given by

$$[Y; Z]_g(f) = Y_g\big(Z(f)\big) - Z_g\big(Y(f)\big) \ ,$$

where $Y, Z \in \mathfrak{l}$, $g \in \mathcal{G}$ and $f \in C_g^\infty(\mathcal{G})$; this function satisfies the skew-symmetry property and the Jacobi identity.

B.2.6 Lemma : *Let $\mathcal{G}$ be a Lie group, e its neutral element, $\mathfrak{g}$ its Lie algebra and $\mathrm{T}_e\mathcal{G}$ its tangent space at e. The map $\mathfrak{g} \to \mathrm{T}_e\mathcal{G}$ sending each $Y \in \mathfrak{g}$ to its value $Y_e \in \mathrm{T}_e\mathcal{G}$ is a linear isomorphism.*

B.2.7 Remark : This isomorphism is so natural that it is often neglected and what is called Lie algebra of a Lie group $\mathcal{G}$ is simply the tangent space $\mathrm{T}_e\mathcal{G}$ furnished with the induced bracket operation.

B.2.8 Definition : A *subalgebra* $\mathfrak{h}$ of a Lie algebra $\mathfrak{g}$ is a Lie algebra which is contained in $\mathfrak{g}$. This means that $\mathfrak{h}$ is a vector subspace of $\mathfrak{g}$ which is closed under the bracket operation.

B.2.9 Definition : A *Lie algebra homomorphism* is a linear map between two Lie algebras preserving the bracket operation.

B.2.10 Example : The Lie algebra of $\mathrm{GL}_n(\mathbb{R})$ is the set of all real $n \times n$ matrices $\mathrm{M}_n(\mathbb{R})$; to be precise, $\mathrm{M}_n(\mathbb{R})$ is (canonically) isomorphic to the Lie algebra of $\mathrm{GL}_n(\mathbb{R})$. This result is a consequence of the fact that the tangent spaces to $\mathrm{GL}_n(\mathbb{R})$ and $\mathrm{M}_n(\mathbb{R})$ at the identity matrix point are identical. The set $\mathrm{O}_n(\mathbb{R})$ of (real) orthogonal $n \times n$ matrices is a Lie subgroup of $\mathrm{GL}_n(\mathbb{R})$; its Lie algebra $\mathfrak{o}_n(\mathbb{R})$ is the set of all $n \times n$ real skew-symmetric matrices. It is a subalgebra of $\mathrm{M}_n(\mathbb{R})$.

B.2.11 Notation : The Lie algebra of $\mathrm{GL}_n(\mathbb{R})$ is also noted $\mathfrak{gl}_n(\mathbb{R})$.

B.2.12 Remark : The previous results can be extended to invertible complex matrices.

B.3   The Lie Exponential Map

B.3.1 Definition : Let $(\mathcal{G}; \diamond)$ be a Lie group. A *one-parameter subgroup* in $\mathcal{G}$ is a smooth homomorphism γ from the group $(\mathbb{R}; +)$ and $(\mathcal{G}; \diamond)$. In other words, $\gamma : \mathbb{R} \to \mathcal{G}$ is a curve such that $\gamma(t_1 + t_2) = \gamma(t_1) \diamond \gamma(t_2)$, for all $t_1, t_2 \in \mathbb{R}$.

B.3.2 Definition : Let Y be a vector field on a Lie group $\mathcal{G}$ and I an interval (in $\mathbb{R}$). A curve $\gamma : I \to \mathcal{G}$ is an integral curve of Y in $\mathcal{G}$ provided that $\dot{\gamma}(t) = Y_{\gamma(t)}$, for all $t \in I$. It is maximal if it cannot be extended to an interval $\tilde{I} \supset I$.

B.3.3 Lemma : *Let $\mathcal{G}$ be a Lie group and $\mathfrak{g}$ its Lie algebra. The one-parameter subgroups of $\mathcal{G}$ are the maximal integral curves of the elements of $\mathfrak{g}$, which start at the neutral element $e \in \mathcal{G}$.*

B.3.4 Definition : Let $\mathcal{G}$ be a Lie group, $\mathfrak{g}$ its Lie algebra, Y an element of $\mathfrak{g}$ and γ_Y the one-parameter subgroup of Y. The *Lie exponential map* is the function

$$\begin{aligned} \exp : \quad \mathfrak{g} \quad &\longrightarrow \quad \mathcal{G} \\ Y \quad &\longmapsto \quad \gamma_Y(1) \ . \end{aligned}$$

B.3.5 Remark : For a fixed $Y \in \mathfrak{g}$, $\exp(tY) = \gamma_{tY}(1) = \gamma_Y(t)$. Thus, exp carries lines through the origin $0 \in \mathfrak{g}$ to one-parameter subgroups of $\mathcal{G}$. Moreover, it is a diffeomorphism between some neighbourhood of 0 in $\mathfrak{g}$ and a neighbourhood of e in $\mathcal{G}$.

B.3.6 Example : In the case of $\mathrm{GL}_n(\mathbb{R})$ (and also $\mathrm{GL}_n(\mathbb{C})$), the Lie exponential map $\exp : \mathfrak{gl}_n(\mathbb{R}) \to \mathrm{GL}_n(\mathbb{R})$ is the usual exponential function given by its power series :

$$\exp A = \sum_{j=0}^{\infty} \frac{A^k}{k!} = I_n + A + \frac{A^2}{2} + \ldots + \frac{A^n}{n!} + \ldots$$

where $A \in \mathrm{GL}_n(\mathbb{R})$; hence the name *exponential*. This also holds for any subgroup of $\mathrm{GL}_n(\mathbb{R})$, for instance $\mathrm{O}_n(\mathbb{R})$.

Appendix C

The Schwartz Space

Main definitions and results are exposed without proofs. More information can be found in the textbooks of L. Schwartz [Sch66], H. L. Royden [Roy68], R. Strichartz [Str94] and S. D. Chatterji [Cha97a, Cha97b], for instance.

C.1 Generalities

C.1.1 Notation : Let $\varsigma \in \mathbb{N}^n$. Then $\varsigma = (\varsigma_1; \ldots; \varsigma_n)$, where $\varsigma_j \in \mathbb{N}$, for all $1 \leqslant j \leqslant n$. We note :

$$\varsigma! = \prod_{j=1}^{n} \varsigma_j! \quad , \qquad |\varsigma| = \sum_{j=1}^{n} \varsigma_j$$

and :

$$\mathrm{D}^\varsigma = \frac{\partial^{\varsigma_1}}{(\partial r^1)^{\varsigma_1}} \frac{\partial^{\varsigma_2}}{(\partial r^2)^{\varsigma_2}} \cdots \frac{\partial^{\varsigma_n}}{(\partial r^n)^{\varsigma_n}} \quad ,$$

where $(r^1; \ldots; r^n)$ are the n (natural) coordinates of $\mathbb{R}^n$, corresponding here to n variables.

C.1.2 Definition : The space of all *rapidly decreasing* smooth functions $f : \mathbb{R}^n \to \mathbb{C}$ on $\mathbb{R}^n$ is called *Schwartz space* and is noted $\mathcal{SCH}(\mathbb{R}^n)$. In other words, $f \in \mathcal{SCH}(\mathbb{R}^n)$ if and only if $f \in C^\infty(\mathbb{R}^n)$ and :

$$[f]_{m,\varsigma} = \left\| (1 + \|r\|^m) \, \mathrm{D}^\varsigma f \right\|_{\mathcal{L}^\infty} = \sup_{r \in \mathbb{R}^n} \left\{ (1 + \|r\|^m) \, |\mathrm{D}^\varsigma f(r)| \right\} < \infty \ .$$

C.1.3 Remark : 1 – Let $f_1, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$ and $a, b \in \mathbb{R}$. Then $a \, f_1 + b \, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$ and $f_1 \, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$, hence the Schwartz space has the structure of an algebra.
2 – If $f \in \mathcal{SCH}(\mathbb{R}^n)$ and P is a polynome, then $P(f) \in \mathcal{SCH}(\mathbb{R}^n)$.
3 – If $f \in \mathcal{SCH}(\mathbb{R}^n)$, $A \in \mathrm{GL}_n(\mathbb{R})$ and $b \in \mathbb{R}$, then the function $r \mapsto f(A \, r + b)$ is also an element of $\mathcal{SCH}(\mathbb{R}^n)$.

C.1.4 Definition : Let $f_1, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$. The function $f_1 * f_2$ given by

$$(f_1 * f_2)(r) = \int_{\mathbb{R}^n} f_1(r - r') \, f_2(r') \, \mathrm{d}^n r'$$

is called *convolution product* of f_1 and f_2. Note that it is symmetric, $f_1 * f_2 = f_2 * f_1$.

C.1.5 Remark : Let $f_1, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$. Then $f_1 * f_2 \in \mathcal{SCH}(\mathbb{R}^n)$. Therefore, the Schwartz space is also an algebra with respect to the convolution product.

C.1.6 Lemma : *Let $f_1, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$. We define :*

$$\langle f_1 \,;\, f_2 \rangle = \int_{\mathbb{R}^n} f_1(r)\, f_2(r)\, \mathrm{d}^n r \;.$$

Then $\langle \;\; ; \;\; \rangle$ is a scalar product and $\langle f_1 \,;\, f_2 \rangle < \infty$.

C.1.7 Remark : In all calculations involving integrals, Lebesgue's definition is meant. Thus, any function f is in fact an equivalence class of functions, the equivalence relation being defined as follows : two functions are equivalent if they differ only on a set of zero measure (for more details, see chapters 3 and 4 in the textbook [Roy68]). The concept of equivalence classes of function is moreover necessary in order to guarantee that $\langle \;\; ; \;\; \rangle$ be positive-definite.

C.2   Tempered Distributions

C.2.1 Definition : The set of all linear functionals on $\mathcal{SCH}(\mathbb{R}^n)$

$$\begin{aligned} \sigma : \mathcal{SCH}(\mathbb{R}^n) &\longrightarrow &\mathbb{C} \\ f &\longmapsto &\sigma(f) < \infty \end{aligned}$$

is called *dual space* of $\mathcal{SCH}(\mathbb{R}^n)$ and is noted $\mathcal{SCH}'(\mathbb{R}^n)$. Elements of $\mathcal{SCH}'(\mathbb{R}^n)$ are called *tempered distributions*.

C.2.2 Definition : A function such that

$$|f(r)| \leqslant c\,(1 + \|r\|^m) \;, \quad \forall\, r \in \mathbb{R}^n \;,$$

where $c > 0$ is a real constant and $m \in \mathbb{R}$, is called *slowly increasing* function.

C.2.3 Remark : Thanks to the scalar product $\langle \;\; ; \;\; \rangle$, there is a linear functional $\sigma_{f_1} = \langle f_1 \,;\;\; \rangle$ for each slowly increasing function $f_1 \in \mathcal{SCH}(\mathbb{R}^n)$; the property of slow increase is necessary to guarantee that

$$\sigma_{f_1}(f_2) = \int_{\mathbb{R}^n} f_1(r)\, f_2(r)\, \mathrm{d}^n r < \infty \;.$$

The reciprocal is not true; there is not necessarily a function for any linear functional σ. In this case, by analogy with tempered distributions associated with slowly increasing functions, we define an element $\tilde{\sigma}$ called *generalised function* such that

$$\begin{aligned} \sigma = \langle \tilde{\sigma} \,;\;\; \rangle : \;\; \mathcal{SCH}(\mathbb{R}^n) &\longrightarrow &\mathbb{C} \\ f &\longmapsto &\langle \tilde{\sigma} \,;\, f \rangle \;, \end{aligned}$$

and :

$$\sigma(f) = \int_{\mathbb{R}^n} \tilde{\sigma}(r) \, f(r) \, \mathrm{d}^n r \ ,$$

where $f \in \mathcal{SCH}(\mathbb{R}^n)$.

C.2.4 Example : Let $\delta_a : \mathcal{SCH}(\mathbb{R}^n) \to \mathbb{C}$, $a \in \mathbb{R}^n$, be the distribution such that :

$$\delta_a(f) = f(a) \ ,$$

where $f \in \mathcal{SCH}(\mathbb{R}^n)$. The associated generalised function $\tilde{\delta}_a$ is such that :

$$f(a) = \delta_a(f) = \int_{\mathbb{R}^n} \tilde{\delta}_a(r) \, f(r) \, \mathrm{d}^n r \ ,$$

implying that it is zero for all $r \neq a$. Since a function which is non-zero only at one point is equivalent to the zero function, its Lebesgue integral should be equal to zero, whereas the definition of the distribution δ_a shows that it is not the case. Thus, $\tilde{\delta}_a$ is not a function in the usual meaning.

C.2.5 Notation : The generalised function $r \mapsto \tilde{\delta}_a(r)$ associated with the distribution δ_a is also noted :

$$r \longmapsto \delta_a(r) = \delta(r - a) \ .$$

The same notation for the generalised function and for the distribution does not create any conceptual problem.

C.3   Fourier Transform

C.3.1 Definition : The *Fourier transform* is the operator $\mathcal{F} : \mathcal{SCH}(\mathbb{R}^n) \to \mathcal{SCH}(\mathbb{R}^n)$ such that :

$$(\mathcal{F}f)(k) = \int_{\mathbb{R}^n} f(r) \exp(\mathrm{i}\, k \cdot r) \, \mathrm{d}^n r \ ,$$

where $k \cdot r = \sum_{i,j=1}^n \delta_{ij} k^i \, r^j = \sum_{j=1}^n k_j \, r^j$ (with $k_j = k^j$, for all $l \leqslant j \leqslant n$).

C.3.2 Notation : The Fourier transform $\mathcal{F}$ of a function f is also noted $\hat{f}$.

C.3.3 Remark : $\mathcal{F}$ effectively carries a function of $\mathcal{SCH}(\mathbb{R}^n)$ to a function of $\mathcal{SCH}(\mathbb{R}^n)$.

C.3.4 Proposition : $\mathcal{F}$ *is well defined, linear, continuous and bijective (one-to-one). Its inverse $\mathcal{F}^{-1}$ is also continuous and is given by* :

$$(\mathcal{F}^{-1}f)(r) = \frac{1}{(2\,\pi)^n} \int_{\mathbb{R}^n} f(k) \exp(-\mathrm{i}\, k \cdot r) \, \mathrm{d}^n k$$

C.3.5 Notation : The inverse Fourier transform $\mathcal{F}^{-1}$ of a function f is also noted $\check{f}$.

C.3.6 Properties : Let $f, f_1, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$, $A \in \mathrm{GL}_n(\mathbb{R})$ and $b \in \mathbb{R}^n$.

1. $\mathcal{F}(f_1 * f_2) = (\mathcal{F}f_1)(\mathcal{F}f_2)$. Indeed :

$$
\begin{aligned}
\big(\mathcal{F}(f_1 * f_2)\big)(k) &= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f_1(r - r')\, f_2(r')\, \mathrm{d}^n r'\, \exp(\mathrm{i}\, k \cdot r)\, \mathrm{d}^n r = \\[2mm]
&= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f_1(r - r')\, f_2(r')\, \exp(\mathrm{i}\, k \cdot r)\, \mathrm{d}^n r'\, \mathrm{d}^n r = \\[2mm]
&= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f_1(\tilde{r})\, f_2(r')\, \exp\big(\mathrm{i}\, k \cdot (\tilde{r} + r')\big) \mathrm{d}^n r'\, \mathrm{d}^n \tilde{r} = \\[2mm]
&= \int_{\mathbb{R}^n} f_1(\tilde{r})\, \exp(\mathrm{i}\, k \cdot \tilde{r})\, \mathrm{d}^n \tilde{r} \int_{\mathbb{R}^n} f_2(r')\, \exp(\mathrm{i}\, k \cdot r')\, \mathrm{d}^n r' = \\[2mm]
&= (\mathcal{F}f_1)(k)\, (\mathcal{F}f_2)(k)\ .
\end{aligned}
$$

2. $\mathcal{F}(f_1\, f_2) = (2\,\pi)^n\, (\mathcal{F}f_1) * (\mathcal{F}f_2)$. The proof is similar to the derivation above.

3. $\big(\mathcal{F}(\partial_j f)\big)(k) = -\mathrm{i}\, k_j\, (\mathcal{F}f)(k)$, for all $k \in \mathbb{R}^n$.

4. $\mathcal{F}\bar{f} = (2\,\pi)^n\, \overline{\mathcal{F}^{-1}f}$, where $\bar{f}(r)$ is the complex conjugate of $f(r)$.

5. If T_b is the operator such that $(T_b f)(r) = f(r + b)$, for all $r \in \mathbb{R}^n$, then :

$$
\big(\mathcal{F}(T_b f)\big)(k) = \exp(-\mathrm{i}\, k \cdot b)\, (\mathcal{F}f)(k)\ ,
$$

for all $k \in \mathbb{R}^n$. Indeed :

$$
\begin{aligned}
\big(\mathcal{F}(T_b f)\big)(k) &= \int_{\mathbb{R}^n} f(r + b)\, \exp(\mathrm{i}\, k \cdot r)\, \mathrm{d}^n r = \\[2mm]
&= \int_{\mathbb{R}^n} f(\tilde{r})\, \exp\big(\mathrm{i}\, k \cdot (\tilde{r} - b)\big)\, \mathrm{d}^n \tilde{r} = \\[2mm]
&= \exp(-\mathrm{i}\, k \cdot b) \int_{\mathbb{R}^n} f(\tilde{r})\, \exp(\mathrm{i}\, k \cdot \tilde{r})\, \mathrm{d}^n \tilde{r} = \\[2mm]
&= \exp(-\mathrm{i}\, k \cdot b)\, (\mathcal{F}f)(k)\ .
\end{aligned}
$$

6. $\big(\mathcal{F}(f \circ A)\big)(k) = |\det A^{-1}|\, (\mathcal{F}f)\big({}^{\mathrm{t}}(A^{-1})\, k\big)$. Indeed :

$$
\begin{aligned}
\big(\mathcal{F}(f \circ A)\big)(k) &= \int_{\mathbb{R}^n} f(A\, r)\, \exp(\mathrm{i}\, k \cdot r)\, \mathrm{d}^n r = \\[2mm]
&= \int_{\mathbb{R}^n} f(\tilde{r})\, \exp\big(\mathrm{i}\, k \cdot (A^{-1}\, \tilde{r})\big)\, |\det A^{-1}|\, \mathrm{d}^n \tilde{r} = \\[2mm]
&= \int_{\mathbb{R}^n} f(\tilde{r})\, \exp\big(\mathrm{i}\, ({}^{\mathrm{t}}(A^{-1}))\, k \cdot \tilde{r}\big)\, |\det A^{-1}|\, \mathrm{d}^n \tilde{r} = \\[2mm]
&= |\det A^{-1}|\, (\mathcal{F}f)\big({}^{\mathrm{t}}(A^{-1})\, k\big)\ ,
\end{aligned}
$$

as $\mathrm{d}^n r = \det A^{-1}\, \mathrm{d}^n \tilde{r}$ and $k \cdot r = {}^{\mathrm{t}}k\, r = {}^{\mathrm{t}}k\, (A^{-1}\, \tilde{r}) = {}^{\mathrm{t}}\big({}^{\mathrm{t}}(A^{-1})\, k\big)\, \tilde{r} = \big({}^{\mathrm{t}}(A^{-1})\, k\big) \cdot \tilde{r}$.

C.3.7 Definition : Let $f_1, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$. We define :

$$(f_1 \mid f_2) = \int_{\mathbb{R}^n} f_1(r) \, \bar{f}_2(r) \, \mathrm{d}^n r \ ,$$

where $\bar{f}_2(r)$ is the complex conjugate of $f_2(r)$.

C.3.8 Lemma : $(\ \mid\ )$ *is a scalar product and* $\big(\mathcal{SCH}(\mathbb{R}^n)\,;\,(\ \mid\ )\big)$ *is a pre-Hilbert space.*

C.3.9 Properties : Let $f_1, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$.

1. $(\mathcal{F} f_1 \mid f_2) = (2\,\pi)^n \, (f_1 \mid \mathcal{F}^{-1} f_2)$. Indeed :

$$
\begin{aligned}
(\mathcal{F} f_1 \mid f_2) &= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f_1(r) \exp(\mathrm{i}\, k \cdot r) \, \mathrm{d}^n r \, \bar{f}_2(k) \, \mathrm{d}^n k \ = \\[2mm]
&= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f_1(r) \, \bar{f}_2(k) \exp(\mathrm{i}\, r \cdot k) \, \mathrm{d}^n k \, \mathrm{d}^n r \ = \\[2mm]
&= \int_{\mathbb{R}^n} \int_{\mathbb{R}^n} f_1(r) \, \overline{\bar{f}_2(k) \exp(-\mathrm{i}\, r \cdot k)} \, \mathrm{d}^n k \, \mathrm{d}^n r \ = \\[2mm]
&= (2\,\pi)^n \, (f_1 \mid \mathcal{F}^{-1} f_2) \ .
\end{aligned}
$$

2. $(\mathcal{F} f_1 \mid \mathcal{F} f_2) = (2\,\pi)^n \, (f_1 \mid f_2)$; this relation is known as the *Parceval-Plancherel equality*. It is a consequence of the previous calculation :

$$(\mathcal{F} f_1 \mid \mathcal{F} f_2) = (2\,\pi)^n \, \big(f_1 \mid \mathcal{F}^{-1}(\mathcal{F} f_2)\big) \ .$$

C.3.10 Lemma : *Let* $f_1, f_2 \in \mathcal{SCH}(\mathbb{R}^n)$. *Then :*

$$\langle \mathcal{F} f_1 \,;\, f_2 \rangle = \langle f_1 \,;\, \mathcal{F} f_2 \rangle \ .$$

C.3.11 Consequence : The previous lemma gives the possibility to define the Fourier transform of a tempered distribution. If $\sigma \in \mathcal{SCH}'(\mathbb{R}^n)$, then $\mathcal{F}\sigma$ is defined by $\mathcal{F}\tilde{\sigma}$, the Fourier transform of the generalised function $\tilde{\sigma}$ associated with σ :

$$(\mathcal{F}\sigma)(f) = \langle \mathcal{F}\tilde{\sigma} \,;\, f \rangle = \langle \tilde{\sigma} \,;\, \mathcal{F}f \rangle \ ,$$

for any $f \in \mathcal{SCH}(\mathbb{R}^n)$.

C.3.12 Example : Let δ_0 be the Dirac distribution, given by $\delta_0(f) = f(0)$, for any $f \in \mathcal{SCH}(\mathbb{R}^n)$. To this distribution corresponds the generalised function $r \mapsto \delta_0(r)$. Its Fourier transform $\mathcal{F}\delta_0$ is given by :

$$
\langle \mathcal{F}\delta_0 \,;\, f \rangle = \langle \delta_0 \,;\, \mathcal{F}f \rangle = (\mathcal{F}f)(0) = \int_{\mathbb{R}^n} f(r) \exp(\mathrm{i}\, 0 \cdot r) \, \mathrm{d}^n r = \int_{\mathbb{R}^n} f(r) \, \mathrm{d}^n r =
$$

$$
= \int_{\mathbb{R}^n} f_{=1}(r) \, f(r) \, \mathrm{d}^n r = \langle f_{=1} \,;\, f \rangle \ .
$$

where f is any function of $\mathcal{SCH}(\mathbb{R}^n)$ and $f_{=1} : r \mapsto 1$ is the constant function equal to 1.

C.3.13 Remark : Neither δ_0 nor $f_{=1}$ belong to $\mathcal{SCH}(\mathbb{R}^n)$. This fact shows the power of the theory of distributions : even functions which do not belong to the Schwartz space can be considered and their Fourier transform can be calculated.

C.3.14 Example : Let δ_Λ be the distribution, the associated generalised function of which is

$$r \longmapsto \delta_\Lambda(r) = \sum_{\lambda \in \mathbb{Z}^n} \delta(r - B\,\lambda) \; ,$$

where $B \in \mathrm{GL}_n(\mathbb{R})$. Its Fourier transform is given by :

$$\langle \mathcal{F}\delta_\Lambda \,;\, f \rangle = \langle \delta_\Lambda \,;\, \mathcal{F}f \rangle = \int_{\mathbb{R}^n} \delta_\Lambda \int_{\mathbb{R}^n} f(r) \exp(\mathrm{i}\,k \cdot r)\,\mathrm{d}^n r\,\mathrm{d}^n k =$$

$$= \int_{\mathbb{R}^n} f(r) \sum_{\lambda \in \mathbb{Z}^n} \exp\big(\mathrm{i}\,(B\,\lambda) \cdot r\big)\,\mathrm{d}^n r = \int_{\mathbb{R}^n} f(k) \sum_{\lambda \in \mathbb{Z}^n} \exp\big(\mathrm{i}\,k \cdot (B\,\lambda)\big)\,\mathrm{d}^n k \;.$$

Thus :

$$(\mathcal{F}\delta_\Lambda)(k) = \sum_{\lambda \in \mathbb{Z}^n} \exp\big(\mathrm{i}\,k \cdot (B\,\lambda)\big) \;.$$

As $k \cdot (B\,\lambda) = {}^\mathrm{t}k\,B\,\lambda = {}^\mathrm{t}({}^\mathrm{t}B\,k)\,\lambda$, we can write :

$$\sum_{\lambda \in \mathbb{Z}^n} \exp\big(\mathrm{i}\,k \cdot (B\,\lambda)\big) \;=\; \sum_{\lambda \in \mathbb{Z}^n} \exp\left(\mathrm{i}\,\sum_{j=1}^{n} ({}^\mathrm{t}B\,k)_j\,\lambda^j\right) \;=$$

$$=\; \sum_{\lambda \in \mathbb{Z}^n} \prod_{j=1}^{n} \exp\big(\mathrm{i}\,({}^\mathrm{t}B\,k)_j\,\lambda^j\big) \;=$$

$$=\; \prod_{j=1}^{n} \sum_{\lambda^j \in \mathbb{Z}} \exp\big(\mathrm{i}\,({}^\mathrm{t}B\,k)_j\,\lambda^j\big) \;,$$

and :

$$\exp\big(\mathrm{i}\,({}^\mathrm{t}B\,k)_j\,\lambda^j\big) = \int_{\mathbb{R}} \delta\big(r^j - \lambda^j\big) \exp\big(\mathrm{i}\,({}^\mathrm{t}B\,k)_j\,r^j\big)\,\mathrm{d}r^j \;,$$

where $r^j \mapsto \delta_{\lambda^j}(r^j) = \delta(r^j - \lambda^j)$ is a generalised Dirac function of a one-dimensional variable. We are then reduced to a calculation involving functions in $\mathcal{SCH}(\mathbb{R})$ and distribution in $\mathcal{SCH}'(\mathbb{R})$. Since $\sum_{\lambda^j \in \mathbb{Z}} \delta_{\lambda^j}$ is periodic, it can be developed into a Fourier series :

$$\sum_{\lambda^j \in \mathbb{Z}} \delta\big(r^j - \lambda^j\big) = \sum_{\ell_j \in \mathbb{Z}} \exp(2\,\pi\,\mathrm{i}\,\ell_j\,r^j)$$

hence :

$$\sum_{\lambda^j \in \mathbb{Z}} \exp\big(\mathrm{i}\,({}^\mathrm{t}B\,k)_j\,\lambda^j\big) \;=\; \sum_{\ell_j \in \mathbb{Z}} \int_{\mathbb{R}} \exp(2\,\pi\,\mathrm{i}\,\ell_j\,r^j)\exp\big(\mathrm{i}\,({}^\mathrm{t}B\,k)_j\,r^j\big)\,\mathrm{d}r^j \;=$$

$$=\; 2\,\pi \sum_{\ell_j \in \mathbb{Z}} \delta\big(({}^\mathrm{t}B\,k)_j - 2\,\pi\,\ell_j\big) \;.$$

Indeed, if we write $k'_j = ({}^t B\,k)_j$, we see that $\int_{\mathbb{R}} \exp(2\,\pi\,\mathrm{i}\,\ell_j\,r^j)\exp(\mathrm{i}\,({}^t B\,k)_j\,r^j)\,\mathrm{d}r^j$ is the Fourier transform $\mathcal{F}\mathrm{pl}$ of the one-dimensional plane wave $r \mapsto \mathrm{pl}(r) = \exp(2\,\pi\,\mathrm{i}\,\ell_j\,r^j)$; a distribution σ_{pl} is associated with this function. The Fourier transform of σ_{pl} acts on any function $f \in \mathcal{SCH}(\mathbb{R})$ as :

$$
\begin{aligned}
(\mathcal{F}\sigma_{\mathrm{pl}})(f) = \sigma_{\mathrm{pl}}(\mathcal{F}f) &= \int_{\mathbb{R}} \exp(2\,\pi\,\mathrm{i}\,\ell_j\,r^j)\,(\mathcal{F}f)(r^j)\,\mathrm{d}r^j = \\
&= \int_{\mathbb{R}} \exp\big(-\mathrm{i}\,(-2\,\pi\,\ell_j)\,r^j\big)\,(\mathcal{F}f)(r^j)\,\mathrm{d}r^j = \\
&= (2\,\pi)\big(\mathcal{F}^{-1}(\mathcal{F}f)\big)(-2\,\pi\,\ell_j) = 2\,\pi\,f(-2\,\pi\,\ell_j) = \\
&= 2\,\pi\,\delta_{-2\,\pi\,\ell_j}(f) \ ;
\end{aligned}
$$

hence $(\mathcal{F}\mathrm{pl})(k'_j) = 2\,\pi\,\delta_{-2\,\pi\,\ell_j}(k'_j) = \delta(k'_j - 2\,\pi\,\ell_j)$. Thus, we have :

$$
\sum_{\lambda\in\mathbb{Z}^n} \exp\big(\mathrm{i}\,k\cdot(B\,\lambda)\big) = \prod_{j=1}^{n}(2\,\pi)\sum_{\ell_j\in\mathbb{Z}} \delta\big(({}^t B\,k)_j - 2\,\pi\,\ell_j\big) = (2\,\pi)^n \sum_{\ell\in\mathbb{Z}^n}\prod_{j=1}^{n} \delta\big(({}^t B\,k)_j - 2\,\pi\,\ell_j\big)\ .
$$

The product of the n one-dimensional generalised Dirac functions corresponds to the n-dimensional Dirac function $k \mapsto \delta({}^t B\,k - 2\,\pi\,\ell)$. Indeed, if we take $\delta_{a^1}\,\delta_{a^2}\ldots\delta_{a^n}$, where $a = (a^1;\,a^2;\,\ldots;\,a^n) \in \mathbb{R}^n$, we have, for any function $f \in \mathcal{SCH}(\mathbb{R}^n)$:

$$
\begin{aligned}
&\int_{\mathbb{R}^n} \delta_{a^1}\,\delta_{a^2}\ldots\delta_{a^n}\,f(r)\,\mathrm{d}^n r = \\
&= \int_{\mathbb{R}}\int_{\mathbb{R}}\ldots\int_{\mathbb{R}} \delta_{a^1}\,\delta_{a^2}\ldots\delta_{a^n}\,f(r^1;\,r^2;\,\ldots;\,r^n)\,\mathrm{d}r^1\,\mathrm{d}r^2\ldots\mathrm{d}r^n = \\
&= \int_{\mathbb{R}}\int_{\mathbb{R}}\ldots\,\delta_{a^1}\,\delta_{a^2}\ldots\int_{\mathbb{R}} \delta_{a^n}\,f(r^1;\,r^2;\,\ldots;\,r^n)\,\mathrm{d}r^n\ldots\mathrm{d}r^2\,\mathrm{d}r^1 = \\
&= \int_{\mathbb{R}}\int_{\mathbb{R}}\ldots\,\delta_{a^1}\,\delta_{a^2}\ldots f(r^1;\,r^2;\,\ldots;\,a^n)\ldots\mathrm{d}r^2\,\mathrm{d}r^1 = \ldots = \\
&= f(a^1;\,a^2;\,\ldots;\,a^n) = \\
&= \int_{\mathbb{R}^n} \delta(r-a)\,f(r)\,\mathrm{d}^n r\ .
\end{aligned}
$$

In $k \mapsto \delta({}^t B\,k - 2\,\pi\,\ell)$, the variables are $k'_j = {}^t B\,k$, $1 \leqslant j \leqslant n$. In order to obtain a function of $k^1,\ldots,k^n$, we need to consider the definition of the generalised Dirac

function; we have :

$$\int_{\mathbb{R}^n} \delta({}^{\mathrm{t}}B\,k - 2\,\pi\,\ell)\,f(k)\,\mathrm{d}^n k \;\; = \;\; \int_{\mathbb{R}^n} \delta\big(k' - 2\,\pi\,\ell\big)\,f\big({}^{\mathrm{t}}(B^{-1})\,k'\big)\,\det B^{-1}\,\mathrm{d}^n k' \;\; =$$

$$= \;\; \det B^{-1}\,f\big(2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell\big) \;\; =$$

$$= \;\; \det B^{-1}\int_{\mathbb{R}^n} \delta\big(k - 2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell\big)\,f(k)\,\mathrm{d}^n k \;\; =$$

$$= \;\; \int_{\mathbb{R}^n} \det B^{-1}\,\delta\big(k - 2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell\big)\,f(k)\,\mathrm{d}^n k\;.$$

In conclusion :

$$(\mathcal{F}\delta_\Lambda)(k) = \;\; (2\,\pi)^n\det B^{-1}\delta_{\Lambda^*}\;,$$

where :

$$\Lambda = \{B\,\lambda \mid \lambda \in \mathbb{Z}^n\}$$

and

$$\Lambda^* = \{2\,\pi\,{}^{\mathrm{t}}(B^{-1})\,\ell \mid \ell \in \mathbb{Z}^n\}\;.$$

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